

Nearly full magnetization recovery after a strong collision between Fe nanoparticles

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The magnetic history of extraterrestrial materials, such as meteorites, is a critical archive for understanding solar system processes. However, the effect of hypervelocity collisions on this record remains poorly understood, particularly whether such events can erase or reset magnetization through heating or pressure-induced phase transformations. Using spin-lattice dynamics simulations, we investigate collisions between nanoscale iron particles (10–20 nm diameter) at velocities of 1–2 km s^{−1}, explicitly modeling magnetic interactions. Our results show that while collisions at 2 km s^{−1} generate pressures sufficient to induce local melting and a limited, transient nonmagnetic hexagonal close-packed (hcp) phase, the primary magnetic effect is global heating above the Curie temperature, transitioning the particles to a paramagnetic state. The particles form a single nanoparticle after the impact, with some twins, dislocations, and point defects. Unlike under bulk single-crystal loading, several nanograins are formed. Upon simulated cooling, emulating radiative cooling, the now-joined particles consistently recover a strong, single-domain ferromagnetic state, irrespective of their initial magnetic-domain orientation or the resulting microstructural defects. The final ferromagnetic state does not preserve a memory of the pre-impact magnetic configuration. These findings demonstrate that a strong ferromagnetic signature in recovered nanoscale iron does not preclude a history of severe hypervelocity collisions, with significant implications for the interpretation of magnetic records in asteroidal and meteoritic materials.

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I. INTRODUCTION

Collisions of nanoparticle (NP) systems and their effect on the magnetic response are an interesting field of research because of their relevance for astrophysics and to possible technological applications of magnetic nanomaterials that might experience impacts.

Regarding bulk materials, impact demagnetization in basalt has been explored experimentally with laser impacts [1]. Magnetization of Fe oxides is also relevant, such as for studies of the primary magnetic mineralogy in the Martian crust [2]. Iron nanoparticle formation in lunar soils is described by diverse mechanisms [3], where micrometeorite impacts and charged-particle irradiation play a significant role, as well as space weathering. These processes produce nanoparticles with sizes in the range of 1–15 nm, which then agglomerate to form structures of hundreds of nanometers. These nanoparticles alter the optical and physical properties of the surfaces of celestial bodies [4].

Numerous works explore collisions of a single NP with a flat surface, including fcc targets [5] and bcc targets like tungsten [6]. Previous studies have investigated collisions of fcc NPs, such as Lennard–Jones NPs [7], Al NPs [8], or AlNi NPs [9]. However, studies on bcc NP impacts appear to be uncommon.

Magnetism has not been taken into account in any of the previous computational studies on NP collisions. We note, however, that Kiwi *et al.* [10,11] have simulated collisions of very small Rh and Au metal clusters (<20 atoms), using spin-polarized density functional theory molecular dynamics (DFT-MD) simulations, lasting 2 ps, to study configurational changes and possible cluster fragmentation. Shocks can magnetize and demagnetize rocks [12], and there are different conditions for ensuring preservation and detectability of shock-induced magnetization [13]. Shock-remanent magnetization (SRM) impacts can impart a new magnetization if they occur in the presence of an ambient magnetic field (e.g., a past core dynamo or the solar-wind field). Shock demagnetization impacts of sufficient intensity can also erase preexisting magnetization by disrupting the magnetic-domain structure of the carrier minerals (e.g., magnetite or iron metal). It is of interest to distinguish between thermoremanent magnetization (TRM) acquired during cooling in strong magnetic fields and secondary shock-remanent magnetization (SRM) from impacts. The natural remanent magnetization of a meteorite is a complex puzzle: it can be a primary TRM from its formation,

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an SRM from a major collision, or a mixture of the two, where a late mild shock partially resets the record. Laboratory shock recovery experiments are essential for calibrating the pressure thresholds for both SRM acquisition and demagnetization in relevant minerals and rocks. For instance, saturation isothermal remanent magnetization as a function of pressure shows large values after compression to 25 GPa followed by decompression for Fe and FeNi alloys [14].

Spin-lattice dynamics (SLD) is an atomistic simulation technique that includes the spin degrees of freedom in the calculation of atomic dynamics. It has been used successfully for around two decades to study the magnetic properties of materials, and in particular Fe. Thus, the effect of point defects and dislocations on the magnetic properties of bulk Fe has been studied [15–19]. Analogous studies were also conducted for nanowires and nanoparticles [20], studying mechanical deformation, domain-wall movement, and twinning. A recent simulation of Fe nanowires with defects from mechanical deformation also included a magnetic domain wall [21].

Given that Fe is such a prominent magnetic material in the cosmos, we considered the case of colliding pure Fe NPs as an initial study, where large pressures can induce a hcp transition leading to the formation of nonmagnetic material [22], as well as large collision temperatures and defect formation that can erase the initial magnetization.

II. METHODOLOGY

While this study focuses on spin-lattice dynamics simulations, we also performed “pure” molecular dynamics (MD) simulations, in which the spin degrees of freedom were ignored, for comparison purposes; these latter simulations will be denoted as “nonmagnetic MD” simulations. All simulations were performed with the software LAMMPS [23], which is open-source and very efficient. To analyze and visualize the data, we used the software OVITO [24].

A. Spin-lattice dynamics simulations

Spin-lattice dynamics simulations were performed using the SPIN package implemented in LAMMPS [25], which extends classical molecular dynamics (MD) by including magnetic degrees of freedom. We note that SLD assumes the electron dynamics to follow adiabatically the atomic motion; this is justified in our case, as the electron Fermi velocity in Fe (1300 km/s) is large compared to atomic velocities considered here ($\lesssim 1$ km/s). This is done by assigning a classical magnetic moment (or spin vector) to each atom in the system. The system Hamiltonian combines atomic and spin contributions as

$$\mathcal{H} = \sum_{i=1}^N \frac{|\mathbf{p}_i|^2}{2m} + \sum_{(ij)} V(r_{ij}) + \mathcal{H}_{\text{mag}}. \quad (1)$$

The first two terms comprise a typical MD Hamiltonian, accounting for the atomic kinetic and potential energies. In these terms, $\mathbf{p}_i$ and m_i are the momentum and mass of atom i , respectively, and $V(r_{ij})$ is the interatomic potential depending on the distance r_{ij} between atoms i and j . The summation runs over all ij pairs without double counting. The last term is the magnetic Hamiltonian, accounting for the magnetic

contributions to the energy. In this work, we have included the following interactions to the magnetic energy:

$$\mathcal{H}_{\text{mag}} = - \sum_{(ij)} J(r_{ij}) \mathbf{s}_i \cdot \mathbf{s}_j - \mathcal{H}_{\text{Néel}}. \quad (2)$$

The first term is a typical Heisenberg Hamiltonian, where $J(r_{ij})$ is the interatomic distance-dependent exchange parameter and $\mathbf{s}_i$ represents classical spin vectors of unit length ($|\mathbf{s}_i| = 1$). The last term represents the Néel anisotropy, which introduces coupling between local lattice distortions and spin orientations. This contribution is crucial for angular-momentum transfer between lattice and spins, and thus for thermal equilibration between both subsystems. In this work, we follow the implementation described by Nieves *et al.* [26],

$$\begin{aligned} \mathcal{H}_{\text{Néel}} = & - \sum_{(ij)}^N g_1(r_{ij}) \left[(\mathbf{e}_{ij} \cdot \mathbf{s}_i)(\mathbf{e}_{ij} \cdot \mathbf{s}_j) - \frac{\mathbf{s}_i \cdot \mathbf{s}_j}{3} \right] \\ & + q_1(r_{ij}) \left[(\mathbf{e}_{ij} \cdot \mathbf{s}_i)^2 - \frac{\mathbf{s}_i \cdot \mathbf{s}_j}{3} \right] \left[(\mathbf{e}_{ij} \cdot \mathbf{s}_j)^2 - \frac{\mathbf{s}_j \cdot \mathbf{s}_j}{3} \right] \\ & + q_2(r_{ij}) [(\mathbf{e}_{ij} \cdot \mathbf{s}_i)(\mathbf{e}_{ij} \cdot \mathbf{s}_j)^3 + (\mathbf{e}_{ij} \cdot \mathbf{s}_j)(\mathbf{e}_{ij} \cdot \mathbf{s}_i)^3], \end{aligned} \quad (3)$$

where $\mathbf{e}_{ij} = (\mathbf{r}_i - \mathbf{r}_j)/|\mathbf{r}_i - \mathbf{r}_j|$ and $g_1(r_{ij})$, $q_1(r_{ij})$, and $q_2(r_{ij})$ are interatomic distance-dependent functions that mediate the intensities of the dipolar and quadrupolar terms. They are given by the following expressions:

$$\begin{aligned} g_1(r_{ij}) &= g(r_{ij}) + \frac{12}{35} q(r_{ij}), \\ q_1(r_{ij}) &= \frac{9}{5} q(r_{ij}), \\ q_2(r_{ij}) &= -\frac{2}{5} q(r_{ij}). \end{aligned} \quad (4)$$

All the interatomic distance-dependent functions $J(r_{ij})$ [Eq. (2)], $g(r_{ij})$, and $q(r_{ij})$ [Eqs. (4)] are defined by a Bethe–Slater function of the form

$$f(r_{ij}) = 4a \left(\frac{r_{ij}}{d} \right)^2 \left[1 - b \left(\frac{r_{ij}}{d} \right)^2 \right] e^{-\left(\frac{r_{ij}}{d} \right)^2} \Theta(R_c - r_{ij}), \quad (5)$$

where $\Theta(R_c - r_{ij})$ is the Heaviside step function and R_c is the cutoff distance. In the case of $J(r_{ij})$, the parameters a , b , and d must be adjusted to fit *ab initio* data. For the Néel spin-lattice coupling, these parameters, for $g(r_{ij})$ and $q(r_{ij})$ in Eqs. (4), can be adjusted following different strategies: (i) they can be tuned to reproduce experimentally observed magnetic properties, like magnetocrystalline anisotropy energy (MAE) [26,27], or (ii) to reproduce the characteristic timescale of the magnon–phonon relaxation [28–30]. In this work, we adopt the second strategy since it enables energy and angular momentum exchange between spins and lattice subsystems within accessible simulation times. The parameters used in this study are given in Table I; the coefficients were obtained by fitting to data by Ma *et al.* [15], cf. Refs. [16,20].

TABLE I. Parameters used for the magnetic interactions.

$f(r_{ij})$	R_c (Å)	a (eV)	b	d (Å)
$J(r_{ij})$	3.5	0.096	0.20	1.54
$g(r_{ij})$	2.6	0.01963735	0.824409	2.4690386
$q(r_{ij})$	2.6	0.00142594	1.05331	2.4690386

The atoms and spins evolve according to the following coupled Langevin equations [25]:

$$\frac{d\mathbf{r}_i}{dt} = \frac{\mathbf{p}_i}{m_i}, \quad (6)$$

$$\frac{d\mathbf{p}_i}{dt} = \sum_{j, i \neq j}^N \left[-\frac{dV(r_{ij})}{dr_{ij}} + \frac{dJ(r_{ij})}{dr_{ij}} \mathbf{s}_i \cdot \mathbf{s}_j \right] \mathbf{e}_{ij} - \frac{\gamma_L}{m_i} \mathbf{p}_i + \boldsymbol{\xi}_i, \quad (7)$$

$$\frac{d\mathbf{s}_i}{dt} = \frac{1}{1 + \lambda_s^2} [(\boldsymbol{\omega}_i + \boldsymbol{\zeta}_i) \times \mathbf{s}_i + \lambda_s \mathbf{s}_i \times (\boldsymbol{\omega}_i \times \mathbf{s}_i)]. \quad (8)$$

The atomic motion follows Eq. (7), where the dynamics are governed by both the interatomic forces and the distance-dependent exchange interaction $J(r_{ij})$. The parameter γ_L denotes the lattice damping coefficient, and $\boldsymbol{\xi}_i(t)$ is a stochastic force drawn from a Gaussian distribution that satisfies the fluctuation–dissipation theorem. The temporal evolution of the spin vectors is described by Eq. (8), with the effective magnetic field acting on spin i given by

$$\boldsymbol{\omega}_i = -\frac{1}{\hbar} \frac{\partial H_{\text{mag}}}{\partial \mathbf{s}_i}. \quad (9)$$

The constant λ_s represents the spin Gilbert damping, and the stochastic field $\boldsymbol{\zeta}_i(t)$ is sampled from a Gaussian distribution. A comprehensive description of the stochastic Langevin formulation and its numerical implementation can be found in Refs. [19,25].

To characterize the magnetic state of the NPs, we calculate the magnetization M as the average magnitude of the spins

$$M = \frac{1}{N} \left| \sum_i \mathbf{s}_i \right| \quad (10)$$

Since the spin vectors are normalized, $M = 1$ in a fully magnetized ferromagnetic state and $M = 0$ in a paramagnetic state at $T \gg T_C$, where T_C is the Curie temperature.

B. Simulation details

1. MD simulation parameters

The following setup was used for all SLD and MD simulations. We considered spherical NPs with diameters d in the range 10–40 nm. The atoms were set in a bcc lattice with lattice parameter $a_0 = 2.8665$ Å, corresponding to the known value for α -Fe. Both NPs were set in the same crystallographic orientation, such that the colliding plane was (001) for both. The orientation of the collision planes is known to influence the elasticity and plasticity of the collision [31]. The results presented are based on the evaluation of a single collision trajectory, in the sense that no ensemble averages were performed. However, the influence of collision parameters—such

as NP velocity, size and orientation—are discussed in the Results section.

We used the embedded-atom method (EAM) potential developed by Gunkelmann *et al.* [32], which provides an accurate description of Fe properties under high-pressure conditions, including a correct description of the bcc–hcp transition. We note that recently, machine-learned (ML) spin-lattice potentials have been developed to study defective magnetic Fe [33]. However, the use of machine-learned potentials is computationally much more expensive (by orders of magnitude) than EAM potentials. In addition, the ML potential has thus far not been tested on its description of phase transformations and plasticity in high-pressure environments.

2. Spin simulation parameters

Regarding SLD simulations, the distance-dependent exchange function $J(r_{ij})$ was parametrized using the same set of parameters reported in Refs. [18,19,34], which accurately reproduce several magnetic properties of bcc Fe, including Curie temperature and magnetic behavior under pressure. The corresponding values of the fitting parameters a , b , and d of Eq. (5) are listed in Table I. This same exchange parameterization was used in a previous SLD work [34] which obtained a Curie temperature for bulk bcc Fe in excellent agreement with the experimental value, $T_C = 1040$ K. In addition, in that work, finite-size effects were found to reduce T_C only for NPs smaller than ~ 8 nm, while larger systems rapidly converge to the bulk limit. A similar size dependence was recently observed for Ni NPs [35]. Although we do not explicitly calculate the critical temperature of the NPs simulated in the present work, the particle sizes considered here (10–40 nm) lie well beyond the regime where surface-to-volume effects significantly modify T_C . Therefore, the Curie temperature of the present NPs is expected to be essentially the same as that of bulk bcc Fe.

For the Néel spin-lattice coupling, the radial functions $g(r_{ij})$ and $q(r_{ij})$, from Eq. (4), were defined following the strategy discussed in the previous section, with the specific parameters given in Table I. With this parameterization for the dipolar and quadrupolar terms of the Néel interaction [see Eqs. (3) and (4)], we end up with a Néel coupling strength 50 times larger than that used by Nieves *et al.* [26]. While such values are appropriate for matching the MAE in bcc Fe, they lead to magnon–phonon coupling times of several nanoseconds, far longer than the subnanosecond dynamics observed in experiments and atomistic simulations. Instead, our objective here is to capture realistic energy transfer between the spin and lattice subsystems; therefore, we adopt a stronger spin-lattice coupling, which results in Néel interaction energies that are ~ 50 times larger than the corresponding values, yielding characteristic magnon–phonon relaxation times of the order of 100 ps, consistent with previous simulations and experimental estimates [28].

This is similar to the strategy employed by Strungaru *et al.* [28], who also utilized a relatively strong Néel-type coupling in order to reproduce sub-100-ps relaxation times. Their choice leads to nearest-neighbor Néel energies of the same order of magnitude as those in the present work. However, as those authors discussed, if the goal were instead to

match the MAE, the Néel coupling would need to be reduced by roughly one to two orders of magnitude, i.e. to values comparable to those of Nieves *et al.* [26]. In that sense, both our parameterization and that of Strungaru's work follow the same logic: enhancing the spin-lattice coupling by a factor of ~ 50 , relative to MAE-fitted values, permits the correct timescale for magnon–phonon equilibration to be captured. As an alternative to the use of a bilinear Hamiltonian for spin-lattice coupling, three-temperature models can be used, with explicit coupling between spin, electron, and lattice temperatures [36–39]. In such models, the spatial dependence of the temperatures is often either neglected or treated within a continuum approach to the heat conduction equation, while SLD directly yields local lattice and spin temperatures.

The total magnetization and each of its components, the magnetic energy and the magnetic temperature, as presented in the work by Nurdin [40], were computed at each simulation step.

For these simulations, we chose a time step of 0.1 fs. Although larger time steps (e.g., 1 fs) have been previously employed in SLD simulations of Fe NPs [19,34], in this work we opted for a smaller time step to mitigate the energy drift arising from the Néel spin-lattice-coupling term.

3. Magnetic moments

The magnitude of the atomic magnetic moments μ is known to depend on the local environment, particularly on the atomic volume, coordination, and/or pressure [41,42]. In the case of nanoparticles, such effects have been approximated using fixed but spatially inhomogeneous moments, for instance by assigning a reduced moment to surface atoms relative to the core, as done in a previous SLD study on Fe core–shell NPs [20]. Other approaches incorporate magneto-volume coupling explicitly. Recently, a tight-binding model, including a Stoner-like term and allowing magnetic moments to vary with atomic volume, was applied to Fe NPs with less than a thousand atoms, which was relaxed using Monte Carlo methods [43]. However, those studies reported an increase in the Curie temperature with decreasing NP size, which contrasts with experimental observations and with previous SLD simulations on Ni NPs [35], where a fixed-moment model yields the expected decrease of T_C with size.

More recently, Nikolov *et al.* [22] developed an SLD framework that includes longitudinal spin fluctuations (LSF), allowing the atomic magnetic moment to evolve self-consistently with local atomic pressure. This approach was used to describe Fe under Earth-core-like pressures and temperatures, where magnetic moments can be substantially reduced or even quenched. However, the local pressures generated during the NP collisions studied here are much lower, and the local pressures and volumes sampled in our simulations remain close to those of bcc Fe. Under these conditions, longitudinal spin fluctuations are not expected to play a dominant role compared to the transfer of angular momentum between the lattice and spins. Furthermore, thermal expansion is generally more pronounced in NPs than in bulk, and the average atomic volume increases as the particle diameter decreases along the collision direction. However, the NPs considered in this work are comparatively large (up to 5.7×10^6

atoms), so the relative change in average atomic volume remains moderate.

In this work, we adopt a constant-moment approximation for all atoms, $\mu = 2.2 \mu_B$, where μ_B denotes the Bohr magneton. This choice neglects longitudinal spin fluctuations, but it allows us to focus on the explicit spin-lattice coupling and energy-angular momentum exchange during collisions. In addition, we use the same magnetic moment for atoms in the crystalline and amorphous (or molten) phases. Several studies show that Fe remains magnetic in disordered phases under moderate densities, with local moments within a comparable range to that of crystalline Fe [44–49]. According to the magneto-volume relation proposed by Ma *et al.* ($M = a \ln V - c + b$) [45], the magnetic moment does not collapse unless the atomic volume is significantly reduced (beyond $\sim 15\%$), which is not the case in our simulations. Additional works relating μ to atomic volume, pressure, or Voronoi coordination [42,48,50] also confirm that under moderate compression or thermal disorder the variation in μ remains within ~ 10 – 20% . Thus, for the conditions studied here, we consider a constant magnetic moment to be a reasonable and computationally efficient approximation.

4. Collision simulations

Two Fe nanoparticles were positioned 1 nm apart. The system was first equilibrated at 100 K by applying independent Langevin thermostats to both the lattice and spin subsystems. This equilibration stage was run for 2 ps, until thermal equilibrium between the two subsystems was reached.

After the relaxation, the collision speed v was defined so that each NP moved towards the other with speed $v_n = v/2$, where $n = 1, 2$ is the index of the NP. Several simulations were performed with collision speeds ranging from 500 m s^{-1} to 2000 m s^{-1} .

During the collision, no Langevin thermostats were applied to either the lattice or the spins, ensuring the conservation of total energy. Collision simulations were carried out in the microcanonical (NVE) ensemble. In the absence of external thermal baths, the temperature of the lattice naturally increased upon impact, and the resulting lattice heating was transferred to the spin subsystem through the spin-lattice coupling terms.

5. Quench

After the collisions, at time $t = 620$ ps, the systems were slowly cooled down to simulate the behavior of a NP in outer space. We expect this material to radiate heat and slowly cool from its high temperature to the average temperature of outer space, around 100 K, as on the equatorial Moon's surface [51]. For this stage, and to mimic radiative cooling, successive SLD simulations were performed using Langevin thermostats, decreasing the target temperature from ~ 800 K to 100 K in steps of 100 K every 12.5 ps. Finally, a 100-ps simulation at 100 K was carried out to ensure the complete relaxation of the lattice and spin degrees of freedom. Therefore, the previous NVE ensemble was replaced by an NVT ensemble, for both subsystems.

By the time the quench starts, the lattice and spin subsystems are in equilibrium, and they remain so, as demonstrated

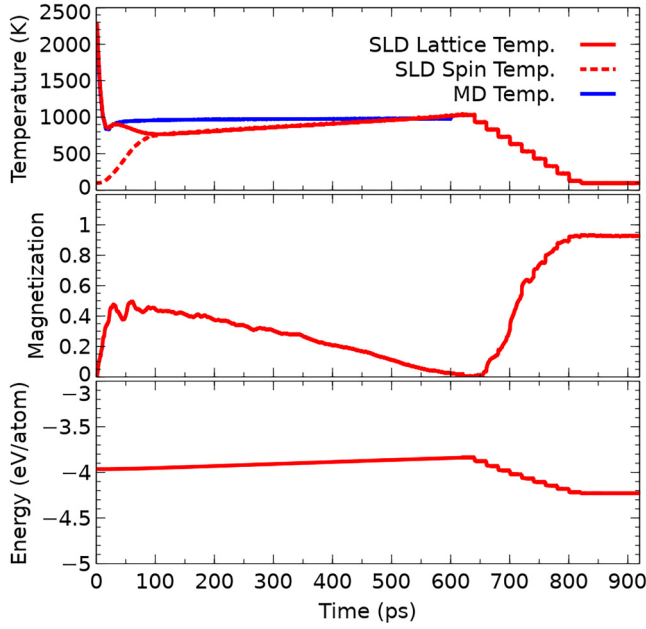


FIG. 1. Temporal evolution of the temperature, magnetization, and energy-per-atom for the SLD simulation. In addition, also the temperature for the nonmagnetic MD simulation is displayed. Data are for a collision of two NPs with $d = 20$ nm at 2 km s $^{-1}$.

by the identical temperature evolution in Fig. 1. Lattice thermalization is extremely fast at the nanoscale [52]. Spin thermalization is somewhat slower, but the evolution of the magnetization during the discrete steps of the quench indicates a good approach to equilibrium. Note that the magnetization at the end of the quench stage remains constant during more than 100 ps after the end of the quench, as also seen in Fig. 1.

6. Data analysis

We used the structure-analysis software OVITO [24] to analyze and visualize the simulations. Dislocation analysis was

performed using the Dislocation eXtraction Algorithm (DXA) as implemented in OVITO [53]. The crystalline structure of the atoms and lattice orientations were identified using the polyhedral template matching (PTM) method [54], which is more reliable than other methods at high anisotropic strain in general, and in particular for NPs under uniaxial strain [55]. The number of grains was computed with the Grain Segmentation tool from OVITO, using a minimum of 7000 atoms per grain. Atomic volume is required to calculate atomic stress, but it is not well defined for surface atoms using Voronoi polyhedra. As an approximation, we assume a constant atomic volume of $a_0^3/2 = 11.8$ Å ^{3} , as appropriate to bulk Fe at zero pressure.

III. RESULTS

A. Spin-lattice dynamics simulation

At first, the simulation results will be presented for the case of the collision of two NPs with $d = 20$ nm at 2000 m s $^{-1}$, in which the two ferromagnetic NPs are magnetized in opposite directions, leading to zero net magnetization. Figure 1 shows the temperature (for both the lattice and spins), the overall magnetization, and the total energy per atom of the magnetic system. At the beginning of the collision, the lattice temperature rises sharply because of kinetic-energy transfer at the impact region, reaching values above the Curie temperature. The collision induces a strong heating of the NP system; after a few tens of ps, the lattice temperature settles at around 1000 K. Energy transfer to the spin subsystem cools the lattice, and after around 100 ps, spin and lattice subsystems have equilibrated at a temperature of around 800 K. An energy drift of around 0.25 eV/atom/ns heats the system at later times; this energy drift is an artifact of the integrator of the spin evolution equations, see Sec. IIIC below. As a consequence of the heating, the system temperature reaches the Curie temperature, and the magnetization drops to zero, indicating a transition to a paramagnetic state. In the

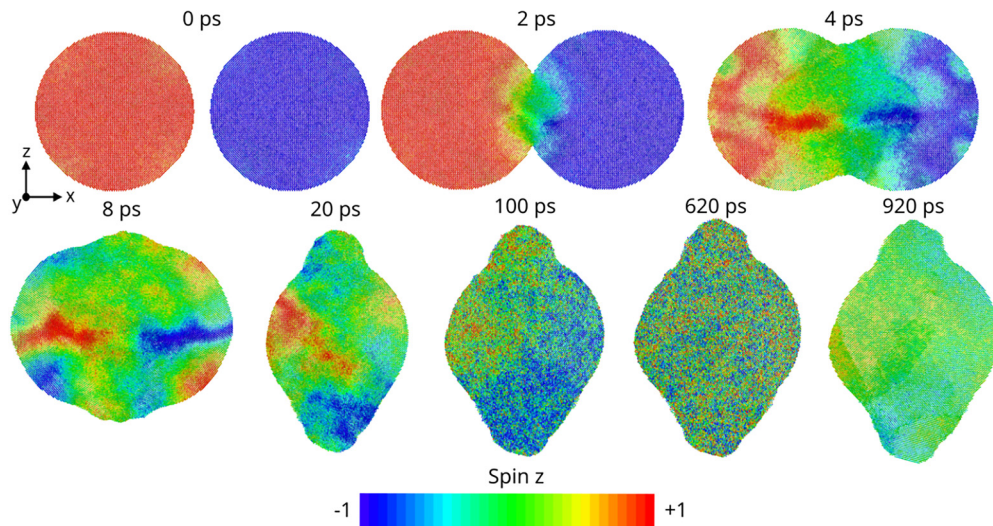


FIG. 2. Spin orientation. Spins are colored with respect to the magnitude in the z direction, perpendicular to the collision axis. Initially, the NPs were polarized along the z axis in opposite directions. At the end of the collision, 620 ps, the domains have vanished and the system has become paramagnetic. After quenching, 920 ps, the collided system consists of a single domain, oriented in the x - y plane.

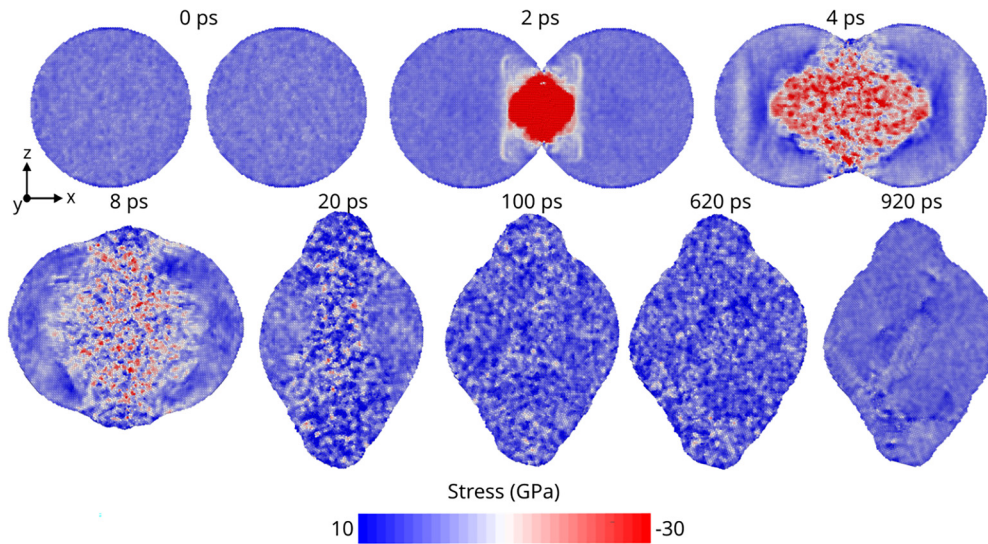


FIG. 3. Hydrostatic atomic stress at various times of the collision. Red coloring corresponds to compressive stress.

quenching phase (620–820 ps), the system is cooled to 100 K, and maintained at this temperature for 100 ps. The system then becomes ferromagnetic again, and the magnetization reaches values close to 1.

The spatial distribution of the spins is depicted in detail in Fig. 2 and allows us to follow the decay of the magnetization in the initially fully magnetized NPs. Concomitant with the deformation of the NPs, the initially well-separated domains (identical to the two NPs) merge, and a complex disordered spin structure is formed. Because of the heating, the system eventually (620 ps) reaches the paramagnetic state. After the quench (920 ps), a single-domain structure again forms, but the magnetization is directed in a different direction, unconnected to the initial magnetization. The average magnetization of the system rotates and changes its magnitude over the course of the simulation. In the first frame of Fig. 2, the magnetization is $0.01 \mu_B$, mostly along y . After 20 ps, it lies in the xy plane, with a magnitude of $0.79 \mu_B$. In the final frame, it is $2.04 \mu_B$, close to the low-temperature bulk value of $2.2 \mu_B$, and lies mostly along x .

Snapshots displaying the spatial distribution of the hydrostatic atomic stress and the local crystalline structure are shown in Figs. 3 and 4, respectively. These snapshots are taken at the same times as the spin distributions shown in Fig. 2. Note that bcc iron undergoes a phase transformation to hcp at a compressive pressure of around 13 GPa, which is well captured by the potential used here [32]; pressures exceeding this value are colored white and red in Fig. 3. The highly compressive stress in the collision zone reaches values of up to 30 GPa, but only for timescales of the order of 10 ps. Indeed, Fig. 4 confirms the formation of small pockets of hcp phase during the period when the high compression is applied; but these pockets decay later with decreasing stress. Also, a few fcc pockets are formed temporarily, as this phase has a comparable enthalpy to that of the hcp phase; but also these pockets are dissolved with decreasing stress. The final structure is characterized by an almost exclusive bcc structure containing a number of lattice defects, identified as “other” types. The term “other” denotes local lattice configurations that PTM cannot match to ideal crystalline environments: the

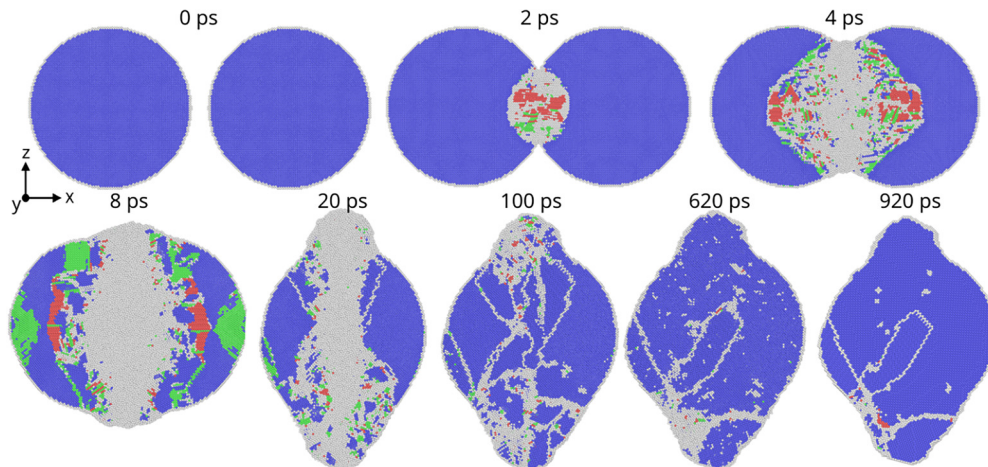


FIG. 4. Local crystalline structures at various times of the collision. Colors correspond to bcc (blue), fcc (green), hcp (red) and other types (gray).

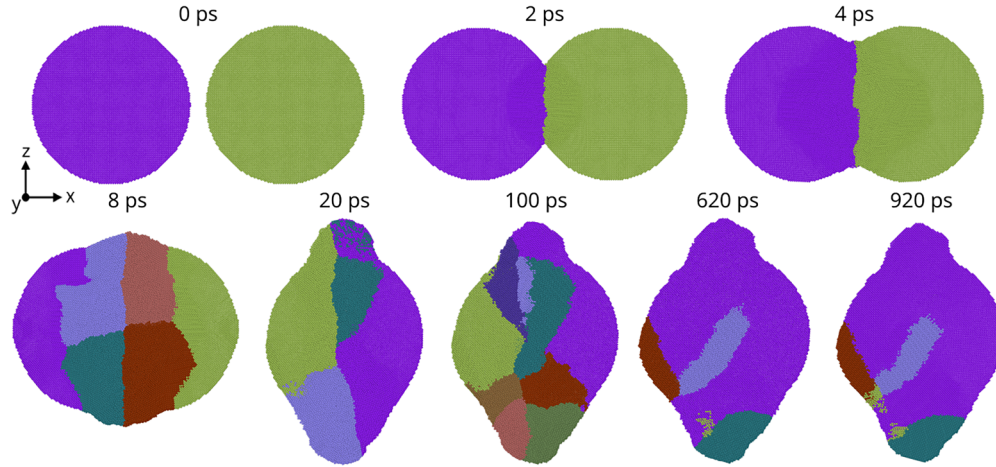


FIG. 5. Subgrain formation. Each color corresponds to a different grain. Only grains containing a minimum of 7000 atoms are shown.

material is locally amorphous—or even temporarily molten—or contains crystal defects in the vicinity of the considered atom, or belongs to a crystal phase not included in the PTM database.

While initially the collision system is composed of two single-crystalline NPs, the collision forms an interesting microstructure through subgrain formation. This process is visualized in Fig. 5. Starting from the high compressive pressures acting during the first 10 ps, the shedding of the NPs into subgrains can be observed; interestingly, this process continues into further grain refinement at later times and will be discussed below.

The strong plastic deformation of the NPs under collision is accompanied and driven by dislocation formation. Figure 6 displays the spatial distribution of the dislocation lines formed. As is common in bcc materials, dislocations with Burgers vector $1/2\langle 111 \rangle$ are most prolific; because of the high speed of the deformation process, also dislocations with longer Burgers vectors— $\langle 100 \rangle$ and even $\langle 110 \rangle$ —are formed, which are energetically less favorable. Figure S1 within the Supplemental Material (SM) [56] demonstrates that screw dislocations abound in the final structure, supplemented by a few shorter edge dislocations.

Finally, we investigated the effect of the Néel anisotropy parameters on the temperature evolution of the system, albeit for smaller NPs, $d = 10$ nm. Figure S2 within the SM [56] shows the effect of the Néel anisotropy parameters on the temperatures of the system. Each curve corresponds to the Néel values reported for bcc Fe [26] multiplied by a constant factor. For a factor of $\times 10$, the spin-lattice temperatures remain weakly coupled. For a factor of $\times 100$, there is strong coupling, but there is a large energy drift for a time step of 0.1 ps. We therefore adopt a factor of $\times 50$ as a compromise between coupling strength and numerical stability.

B. SLD vs MD comparison

To assess the effect of the spins during the collision, we ran a simulation (nonmagnetic MD) with the same setup as described before, but only considering the Fe atoms and neglecting spin degrees of freedom. Figure 1 shows the different evolution of the temperature for both simulations. Because of the coupling to spins, the lattice temperature in SLD is lower than that in nonmagnetic MD. The effective heat capacity of the spin system can be read off these data: it amounts to around $0.75k_B T$ per spin. This value is in good agreement

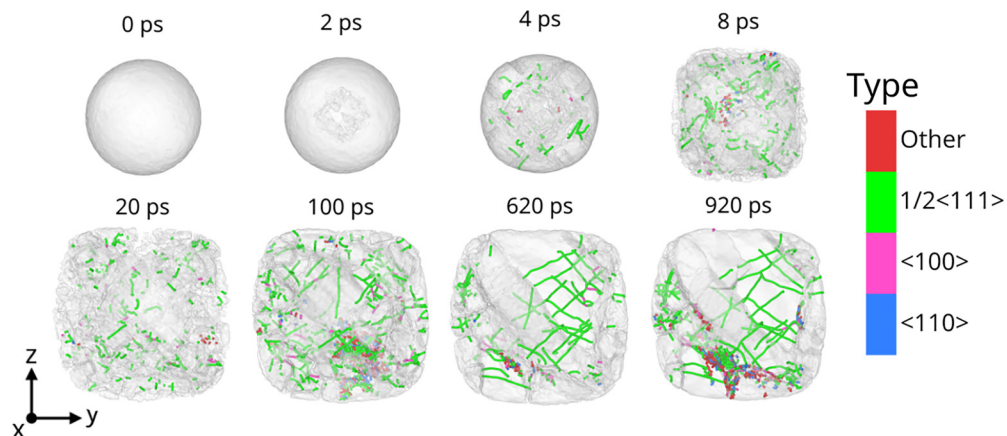


FIG. 6. Dislocation formation, viewed along the collision axis. Dislocations are colored by their Burgers vector, as shown in the color bar.

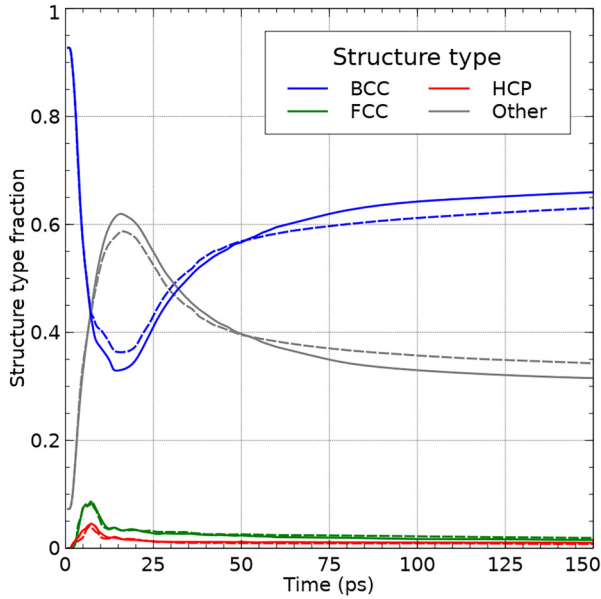


FIG. 7. Structure type fractions for spin-lattice dynamics (solid lines) and molecular dynamics (dashed lines).

with previous simulation results [20,57] as it is well known that the spin heat capacity peaks around the Curie temperature [58–60]. The energy drift of the SLD code is clearly discerned in contrast to nonmagnetic MD. When the collision simulations are stopped, at around 600 ps, both simulations have reached roughly the same lattice temperatures.

The effect of the collision on the phase transformations occurring within the collided NPs is demonstrated quantitatively in Fig. 7. For the SLD simulation, this figure supplements Fig. 4, and the data for the nonmagnetic MD simulation are added. The main conclusion is that the inclusion of spins in the simulation has only a negligible effect on the phase transformations. The close-packed phases hcp and fcc are formed under high pressure, at around 5 ps, but later mostly decay as the pressure relaxes, as expected. It is known that the magnetic moment in the close-packed phases is quenched; while this effect is not included in our (constant-moment) SLD simulations because the close-packed fraction is small and transient, this figure indicates that the magnetic effect on the phase transformations is minor. The significant fraction of “other” crystallographic environments remaining long after the collision is caused by the occurrence of defects such as grain boundaries and dislocations in the collided NP.

These defects are analyzed through their temporal evolution in Figs. 8 and 9, which display the temporal evolution of the number of grains and the total length of dislocation lines formed by the collision, respectively, and compare the SLD and nonmagnetic MD results. Again, a gross agreement in the defect evolution between the two simulations is apparent. Note that defect formation starts immediately after the collision (3–4 ps) and exhibits a maximum at around 5–10 ps, corresponding to the time of maximum compression. Later, as the compression relaxes, at around 20 ps, both the number of subgrains and the dislocation length slightly decrease, but recover again and reach their maximum values at around 100 ps in the relaxation of the hot collided NP, which is strongly out

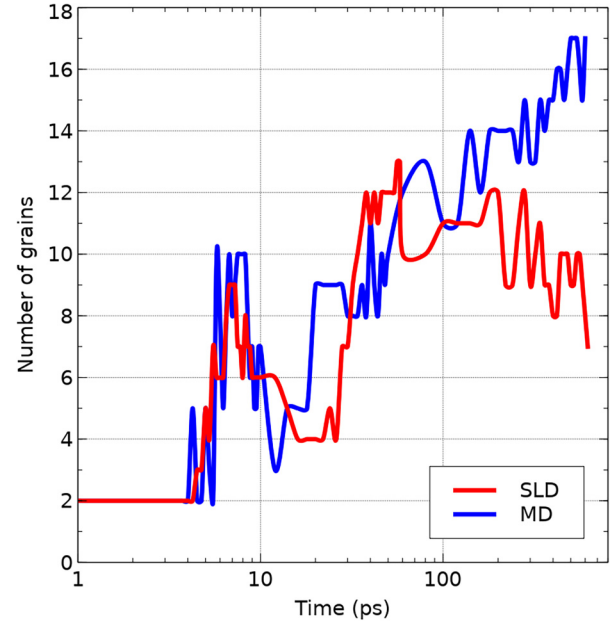


FIG. 8. Grain counts for SLD and MD simulations, considering a minimum grain size of 7000 atoms.

of equilibrium. We argue that the differences in detail seen between the SLD and MD results—in particular, the eventual increase in the number of subgrains in the MD simulation—are caused by fluctuations in the defect-nucleation events. We have verified this by running the same collision but using different random seeds for the Gaussian distribution of velocities. This is a common feature of atomistic simulations of NP collisions, as demonstrated in detail previously [7].

C. Influence of NP size, orientation, and collision speed

The influence of the collision speed v is studied in Fig. 10, which compares the cases $v = 2$ km/s and 1 km/s for smaller

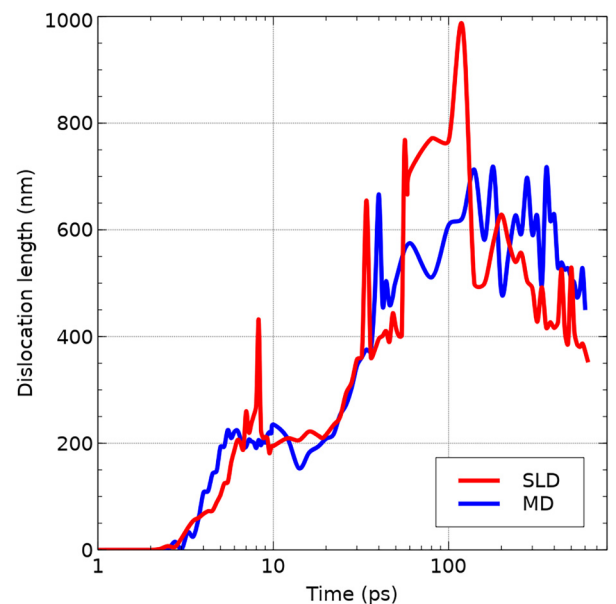


FIG. 9. Dislocation lengths for SLD and MD simulations.

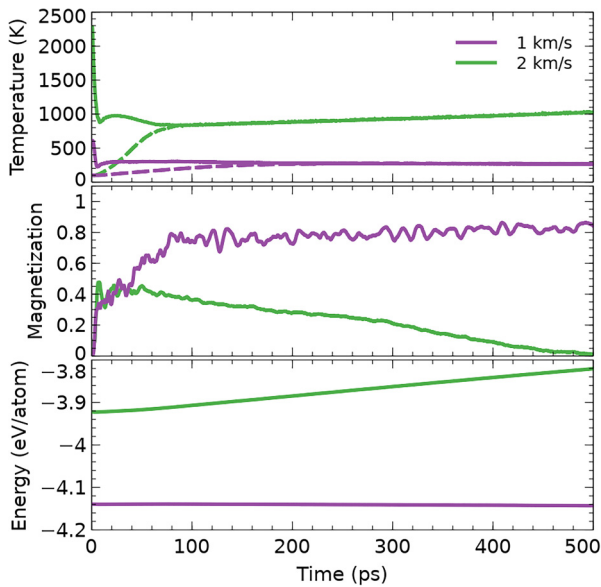


FIG. 10. Temperatures (lattice and spin), magnetization and energy comparison for collisions of NPs with $d = 10$ nm at different speeds.

NPs, $d = 10$ nm. The results for $v = 2$ km/s can be directly compared to those for the larger NPs, $d = 20$ nm, in Fig. 1; close agreement was observed: Spin and lattice temperatures equilibrate at around 100 ps; temperatures around the Curie temperature are reached; consequently, the magnetization drops to values close to zero; the transfer of energy from the lattice to the spin system considerably decreases the lattice temperature; artificial heating increases the temperature on longer timescales. This agreement demonstrates that for these nanosized systems, the temporal evolution after collision is largely independent of particle size.

For a smaller collision velocity, $v = 1$ km/s, the evolution is quite different. Consistent with the collision energy, which is only $1/4$ of that for $v = 2$ km/s, the lattice temperatures reached after the collision only amount to 300 K, i.e., a temperature increase of only $1/4$ of that in the $v = 2$ km/s system. However, energy coupling to the spin system now takes twice as long as for the higher-energy collisions at $v = 2$ km/s. Since the spin temperature is now significantly below the Curie temperature, the system remains ferromagnetic, and the magnetization reaches values of around 0.8 at the end of the simulation.

In order to clarify how quickly spin and lattice systems equilibrate thermally, we performed the following model simulations. In a homogeneous lattice, spin and lattice temperatures were initially set to 100 K. After the lattice temperature was suddenly increased by ΔT , the rate of temperature increase in the spin system, dT_{spin}/dt , was determined. As Fig. S3 within the SM [56] demonstrates, the rate increases linearly with ΔT : large heat differences between the subsystems lead to large heating rates. In addition to this mechanism, the dynamics of the collision may play a role in the rate of energy exchange. Larger impact velocities might lead to increased magnon–phonon scattering, leading to an enhanced magnon–phonon energy exchange, which would couple spin

and lattice temperature faster. Also, an increased impact velocity leads to a larger contact area, and this might provide faster energy exchange between the two NPs.

Note that initially two NPs with opposed magnetic polarization collided; the high value of the final magnetization therefore means that the “domain wall-like” configuration between the NPs vanished. This is shown in Fig. 11, where the spatial distribution of spins at several times after the collision is displayed. For the high velocity, $v = 2$ km/s, the evolution closely parallels that of the larger NPs shown in Fig. 2 and ends with a paramagnetic spin configuration. For the lower velocity, $v = 1$ km/s, the evolution is characterized by strong spatial fluctuations; for instance, at 100 ps, the two NPs seem to almost have inverted their magnetizations. Despite these spatial fluctuations, the total magnetization builds up to the high values reached at around 100 ps and then stays roughly constant; see Fig. 10. We conclude that for collisions in which the temperature remains below the Curie temperature, the collided NP achieves a single-domain ferromagnetic state.

Interestingly, the energy drift for the 1 km/s collision is considerably smaller than for the 2 km/s case. In our experience, the problems with energy conservation in SLD only originate from high spin temperatures and when the Néel term is present. LAMMPS uses the Suzuki–Trotter decomposition to solve the spin equations of motion [25], which might be a reason for the problem.

For nonmagnetic NPs, a series of collisions was performed where the relative orientation of the two colliding NPs was systematically varied. The results—for $v = 2$ km/s and $d = 10$ nm—are displayed in Figs. S10 and S11 within the SM [56]. We find that the final microstructure and plasticity depend on relative orientation, as expected, but the qualitative final states are the same, including dislocations, twins, and point-defects. In our simulations of magnetic NPs, the system reaches temperatures close to the Curie temperature and the spins are oriented randomly. After quenching, a net magnetization appears with a random orientation. We therefore do not expect any major effect of the initial NP orientation on the magnetic structure of the collided NP system.

Finally, we simulated the collision of large NPs with a diameter of $d = 40$ nm (5.7 million atoms in total); these simulations are at the limit of our computational resources, being only possible for nonmagnetic MD, and even then they were terminated after 50 ps. The evolution of the microstructure was followed by monitoring the local crystalline structures, Fig. S4 within the SM [56]. The destruction of the bcc phase and the temporary build-up of defective (other) and close-packed (hcp and fcc) structures closely parallel that for the $d = 20$ nm NP collision shown in Fig. 7. For a quantitative comparison it must be borne in mind that for the NPs with doubled diameter, the passage of compression and release waves through the system—which sets the timescale for the phase transformation to the high-pressure hcp phase, and also for the recovery of the bcc phase—also doubles. For this large system, the evolving microstructure is better visualized than for the smaller systems. We therefore present snapshots of the system highlighting the spatial distribution of crystalline phases (Fig. S5 within the SM [56]) and of the dislocation network formed (Fig. S6 within the SM [56]). Finally, Fig. S7 within the SM [56] displays the shear strain at the end of the

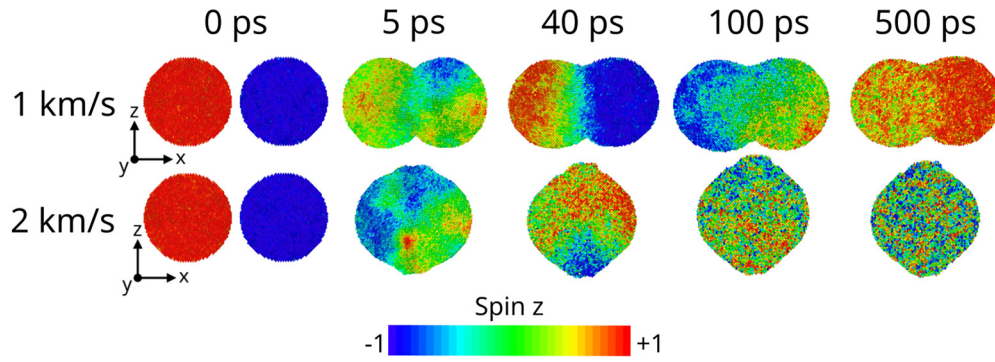


FIG. 11. SLD simulations at different collision speeds for NPs with $d = 10$ nm. We show spins colored with respect to the magnitude in the z direction.

simulation, $t = 50$ ps. Four distinct regions with low strain, related to the four equivalent $\{111\}$ planes for preferential dislocation slip in the bcc lattice compressed along the $[100]$ direction, can be observed.

D. Influence of the initial NP spin orientation

In the simulations considered up to now, the spin orientation of the two colliding NPs was antiparallel; this corresponds to an angle ϕ between the magnetizations of 180° . In this section, we examine to what extent the initial spin orientation can influence the collision dynamics and perform simulations for $\phi = 0^\circ$ (parallel magnetizations) and $\phi = 90^\circ$ (perpendicular magnetizations), as depicted schematically in Fig. 12. These simulations were performed for NPs of diameter $d = 10$ nm at a speed of 2 km/s. Figure 13 demonstrates that the energetics of the collision—as captured by the temporal evolution of the lattice and spin temperatures—are unaffected by the initial orientation. In particular, the time for spin-lattice equilibration is the same in all cases. We take this agreement as evidence that the methodology employed to couple the lattice and spin subsystems works well for arbitrary initial magnetization orientations.

The evolution of the magnetization of the collided NP is displayed in Fig. S8 within the SM [56]. For the antiparallel case, the evolution corresponds to that shown in Fig. 11. The other cases, with parallel and perpendicular initial orientation, show higher magnetizations throughout their evolution; this is caused by the higher initial values of the magnetization resulting from the initial orientations. However, the decays of the magnetization, in particular for later times, parallel each other, as the systems tend toward the paramagnetic phase. An atomistic view of the spatial arrangements of the spins at the end of the simulation is provided in Fig. S9 within the SM [56] (left column) and shows nearly indistinguishable configurations.

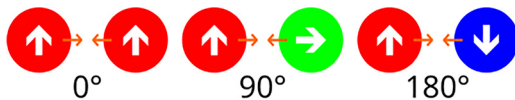


FIG. 12. Schematic diagram showing the initial NP magnetization orientations studied.

In Fig. S9 within the SM [56], we also display the microstructure at the end of the simulation: local crystalline structure (middle column) and dislocations (right column). Some differences in the final microstructure are seen, but they are within what can be expected because of statistical variations in the final outcome, as happens when the initial atomic positions are slightly modified. All these simulations lead to twinning after the collision, but only for $\phi = 90^\circ$ does one of these twins survive at the grain center and help anchor some dislocations that go from the twin interface to the surface. In the other cases, twins disappear, and dislocations are reabsorbed at the surface, except for a single dislocation for $\phi = 0^\circ$, which was previously anchored by a twin and might disappear at longer times. Larger NPs, like the 20-nm-diameter case, lead to more dislocation segments and a more complex dislocation forest, with dislocation junctions that impede dislocation re-absorption at the surfaces, allowing for dislocation survival at long times.

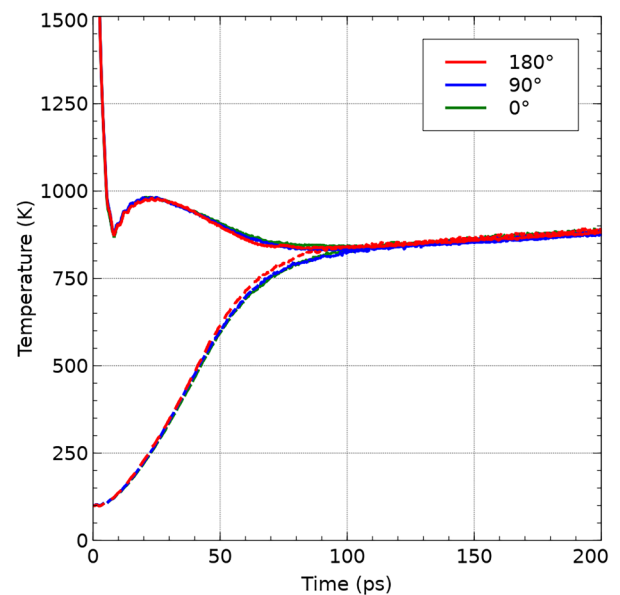


FIG. 13. Lattice and spin temperatures (solid and dashed lines respectively) for different initial NP magnetization orientations.

IV. DISCUSSION

Our simulations focus on nanoscale grains; however, for astrophysical applications, it is important to consider what would happen in the collision of larger grains.

A. Microstructure and formation of close-packed phases

The transformation of Fe under pressure from the bcc to the hcp phase at around 13 GPa is experimentally well characterized [61,62], and so is the concomitant breakdown of magnetization [63].

Shock experiments on bcc Fe indicate that, upon release, Fe largely returns to its bcc structure, with the exception of small regions associated with twin boundaries and/or hcp-related defects [64]. Based on recovered shock microstructures, such studies conclude that dislocation plasticity was scarce during shock loading, whereas deformation twinning accommodates the shock strain, as observed in our NP simulations and bulk MD results. Righi *et al.* [65] show that bcc Fe recovers from hcp very rapidly, with transformation and back transformation times being similar and strain-rate dependent.

In our simulations, there are no significant fractions of the hcp phase, given that the shock-release interval lasts only a few ps. A rough estimate of this interval could be obtained by assuming that the shock velocity is similar to the sound velocity V_s , which is appropriate for weak shocks and would provide a lower limit for stronger shocks. The time required for large hcp contributions would be such that the time required for the shock wave to traverse the diameter D of the target and release is longer than the transformation time. Setting that transformation time t_{tr} to around 10 ns, for a typical strain rate of km/s collisions, and using $V_s = 6$ km/s, gives $D = V_s t_{tr} = 60$ μ m, which, of course, is well beyond atomistic simulation capabilities. However, the qualitative behavior of the magnetization would be similar to our simulations, given that the temperature increase due to the collision will erase the magnetic order within nanosecond timescales, likely before the hcp transition completes.

In our simulations, the pressure drops rapidly to zero, but the lattice temperature is close to 1000 K. A bulk bcc sample under these conditions is close to the bcc–fcc phase transition. The EAM potential we are employing describes this transition reasonably well, but for the cases studied here, the fcc fraction remains small. This issue is relevant since fcc Fe is magnetic, but its exchange interactions have a significantly different dependence on distance, beyond the possible change in magnetic moment [66]. This would have to be revised if there were a large fcc phase fraction.

We therefore conclude that the hcp and fcc fractions formed during bcc Fe NP collisions are transient and not likely to influence the magnetic state of the collided aggregate under the conditions studied.

B. Magnetic structure and formation of magnetic domains

A prime result of our simulations is that the collided NP system assumes a single-domain ferromagnetic state; in the case that the temperature is above the Curie temperature, this single-domain state is reached after quenching.

Above T_C , the material is paramagnetic; there is no long-range magnetic order. As the sample cools through T_C , it undergoes a transition to a ferromagnetic state and may reduce its magnetostatic energy by developing nonuniform magnetization textures. Magnetization time evolution would depend on the ratio of exchange to dipolar interactions. For a 2D Ising system, it was shown to follow a rapid exponential evolution in time [67].

As our simulations are, for computational reasons, restricted to NP sizes of a few tens of nanometers, it is important to discuss how the magnetization state may change for larger colliders. It is well known that larger magnetized Fe crystals are prone to forming domain structures to reduce magnetostatic energy [68,69]. Domain size is governed by the interplay of exchange energy—favoring large domains—and anisotropy energy—penalizing domain walls. In detail, an increase in the effective anisotropy K_{eff} modifies intraparticle domain behavior mainly by changing the characteristic micromagnetic length and energy scales. In particular, the domain-wall width decreases as $\delta \sim \pi \sqrt{A/K_{eff}}$, where A is the exchange energy, while the domain-wall energy increases as $\gamma \sim 4\sqrt{AK_{eff}}$ [69], so higher anisotropy promotes sharper magnetization gradients where nonuniformity occurs, but simultaneously penalizes the formation of multiple walls, favoring fewer-domain states. In Fe nanoparticles in the 10–50-nm range, the dominant effect is frequently a shift in the competition between quasi-uniform configurations and flux-closure textures (for example, curling or vortex-like states), as supported by real-space observations of size-driven single-domain-to-vortex transitions in Fe nanocubes [70].

We conclude that in collisions of Fe NPs larger than those studied here, the effect of magnetic-domain formation needs to be included to reliably model the final (possibly postquench) magnetic state reached.

Here, it should also be noted that the domain structure reached after quenching may depend on the cooling rate. During slow cooling, the system has ample thermal energy and time to nucleate domains at optimal sites (e.g., defects and surfaces) and for these domains to grow and rearrange into a configuration that minimizes the total energy. This typically results in a relatively simple, coarse domain pattern with a lower number of domains and wide domain walls. On the other hand, during rapid cooling, the system is kinetically trapped. The transition through T_C is so fast that there is insufficient time for domain walls to propagate and for the domain pattern to coarsen. This results in the simultaneous nucleation of a vast number of small magnetic domains across the entire volume. The resulting structure is often a complex, fine-scale pattern, sometimes described as a “maze” or “fir-tree” structure, with a very high number of domains. This is analogous to the crystallization of a metal from a melt: slow cooling gives large grains, and rapid quenching gives fine grains.

For the collision of macroscopic Fe bodies, the following picture holds: A typical macroscopic chunk of Fe, which initially has a large magnetization, then is heated above T_C , and finally is cooled well below T_C , will likely form many magnetic domains during cooling. The magnetization direction of these domains will be random in the absence of external magnetic fields. Therefore, the cooled chunk is ferromagnetic,

but it has nearly zero global magnetization, which is typical of a very soft magnet.

We note that very small iron NPs show a superparamagnetic rather than ferromagnetic behavior [71]. Experiments (at 300 K) show that this transition occurs in the range of 10–20 nm for Fe NPs [72–74]. Theoretical considerations demonstrate that the transition is shifted to even smaller NP sizes at lower temperatures [71], since temperature enters the magnetic flip time of a NP as an Arrhenius factor. Hence, the NPs considered in the present study can be considered to be ferromagnetic at a temperature of 100 K.

Impact into magnetized material may form a source for magnetization and demagnetization and has been discussed in this respect in astrophysical contexts. An example is provided by the lunar surface, where it is argued that the cooling of hot impact ejecta in a (previous) dynamo field may have given rise to magnetized crust material, but also that shock and temperature induced by impacts may have induced demagnetization [75]. Our present findings certainly support the first mechanism, in particular in the presence of an external field. However, at least for Fe material, we emphasize that impact-induced high pressures and temperatures are temporary effects that do not lead to lasting effects on the material's magnetization.

Finally, the magnetization of Fe and FeNi crystallites found in meteoritic materials can be discussed in this context. Recently it has been argued that the nanomagnetic properties of small crystallites with sizes of a few tens of nanometers—featuring various domain structures ranging from single-domain states to vortex magnetization and two-domain states—may be connected to the thermal history (slow cooling) of these materials [76].

The simulations performed in this study did not include an external magnetic field. Indeed, such fields would have to be of the order of 60 T for the Zeeman energy to equal the thermal energy (at 100 K). Preliminary simulations, with an external field below 1 T applied during the cooling of the NP, showed no correlation between the direction of the final magnetization and the external field, for the simulated conditions, as expected based on the above. In a previous study of hysteresis for an 8-nm-diameter Fe nanoparticle [19], the field needed for saturation was about 0.15 T at $T = 500$ K, assuming a large anisotropy along the field direction. The coercive field was 0.05 T. This is consistent with some experimental measurements for larger Fe NPs [74]. Therefore, one might expect that the initial magnetization results from thermal fluctuations but, as the particle slowly cools down, it will align with the external magnetic field, for fields larger than the saturation field. For much larger particles, above 50–100 nm, with possible multidomain configurations, the field needed to move domain walls while avoiding pinning by defects will likely be larger than the saturation field for single-domain NPs.

V. SUMMARY AND CONCLUSIONS

We performed spin-lattice-dynamics collisions between two Fe NPs. We systematically varied the impact velocity (1–2 km/s), particle size (10–40 nm diameter), and relative

orientation of the initial magnetizations, and compared SLD against nonmagnetic MD to isolate magnetic effects. This enabled us to obtain insight into the microstructure evolving in the collided aggregate and, in particular, into its magnetic properties. Our main results are as follows.

(1) For collisions in which temperature remains below the Curie temperature, the collided NP achieves a single-domain ferromagnetic state. In the case of more energetic collisions, in which the temperature reaches T_C , the system becomes paramagnetic; after quenching, a single-domain ferromagnetic state is again achieved.

This is certainly the prime result of our study. It could hardly have been reached without applying the SLD methodology as outlined in this study. As discussed in detail in Sec. IV B above, this result holds for the nanosized NPs considered here; larger NPs may develop magnetic domains while maintaining an overall small net magnetization.

(2) Collision results are not influenced by the initial magnetization orientation—obviously apart from the initial values of the magnetization.

(3) Results are largely independent of NP size in the nanometric size regime studied (10–40 nm).

(4) When the spin system reaches temperatures around the Curie temperature, where its heat capacity is large, the lattice temperature is significantly decreased in comparison to that of the nonmagnetic case.

(5) Close-packed Fe phases, such as hcp and fcc, develop only temporarily during the collision; they quickly decay when the pressure relaxes. The development of these phases has no effect on the final fate and magnetization.

Beyond its astrophysical implications, our results on the magnetic response of Fe NPs under high-velocity impacts are linked to several technological applications.

In particular, our findings on the recovery of magnetization after extreme heating are important for ensuring data stability in next-generation storage devices after heating cycles. For instance, in heat-assisted magnetic recording (HAMR) [77], materials undergo rapid thermal cycles above their Curie temperature to overcome magnetic coercivity; the ability of the system to reliably restore its magnetic state is a critical factor for long-term information retention. Furthermore, the microstructural evolution during high-speed collisions provides valuable insights into shock consolidation and cold-spray additive manufacturing [78–80]. In these processes, the final magnetic performance depends on the survival of magnetic properties after severe plastic deformation, a challenge directly addressed by recent efforts to fabricate or repair pure-iron magnetic components via high-velocity impact [81].

In addition, NP collisions are relevant to experiments and models applying high pressure and temperature to NP collections in order to obtain nanopowder compacts [82,83]. This topic is also relevant to low-velocity collisional agglomeration of magnetic nanoparticles, which has been modeled by discrete-element models (DEM) [84]. High-velocity NPs are used to jet-polish surfaces, and an accurate determination of the elastic-plastic transition is necessary [85]. Finally, cluster-beam deposition can be used to generate magnetic NPs, whose evolution will depend on defect content [86].

Future studies will extend our results in several directions. An obvious extension is to try to increase the NP size. While this is computationally demanding, the investigation of the possible occurrence of magnetic final configurations that are not single domain would be rewarding.

A second direction is to perform simulations which allow for modeling variable magnetic moments. These would be necessary for including the different magnetic behavior of surface and bulk Fe atoms [20], and also of fcc, hcp, and bcc Fe domains.

Finally, the extension of the present results to FeNi alloys will be valuable in an astrophysical context. The main problem here—the formulation of the magnetic parameters for modeling—has recently been solved [87]. FeNi NPs will also crystallize in the bcc structure if the Ni content is less than about 15 atomic percent [88]. Larger Ni contents would lead to materials combining both fcc and bcc phases and eventually to predominantly fcc phases, where plastic deformation would proceed through different channels. Magnetic properties of FeNi NPs are complex and depend strongly on NP topology [87].

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

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