

Atomistic calculation of the τ_0 inverse attempt frequency in Fe_3O_4 magnetite nanoparticles

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The Arrhenius law predicts transition times between equilibrium states in thermally activated systems, with broad interdisciplinary relevance. In paleomagnetism, it is used to estimate relaxation times and the thermal stability of magnetic nanoparticles. Magnetite, key to both paleomagnetic studies and magnetic hyperthermia, shows large uncertainties in its attempt frequency f_0 , varying over 10^7 – 10^{13} Hz and affecting relaxation rate estimates. We present a dynamical method using atomistic spin dynamics to fully parametrize the Arrhenius-Néel law. For magnetite nanoparticles with cubic anisotropy, we find $\tau_0 = 0.98 \pm 0.13$ ns at room temperature. For particles with enhanced anisotropy, τ_0 decreases significantly and shows a different temperature dependence, highlighting the role of anisotropy. Our method applies to a broad range of systems with clearly defined states and enables robust estimates of domain stability, with particular relevance for the micromagnetic analysis of paleomagnetic records and improving our understanding of geomagnetic fidelity over geological time.

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I. INTRODUCTION

The Arrhenius law [1] predicts the mean time that an equilibrium state of a physical system is stable before thermal activation overcomes the energy barrier for a transition into another equilibrium state. The law was originally developed in chemistry to explain and determine reaction frequencies in chemical processes [1–3], but due to its simplicity and versatility it is now used across a wide range of disciplines and research areas [4–6]. One example is in nanomagnetism, where the Arrhenius-Néel law [7] can determine the average timescales for transitions between equilibrium magnetization states in magnetic nanocrystals. This is of interest for a wide range of applications such as magnetic recording media [8], medical sciences [9], or paleomagnetism [7]. The attempt frequency is of particular interest in paleomagnetic studies, because it determines the rate at which a magnetic state in a particle attempts to switch to another domain state, and thus is a key factor in determining the stability of ancient recordings of the geomagnetic field. These ancient recordings can tell us about key events during the evolution of the Earth, such as stagnant-lid tectonics during the Hadean and early Archean eons [10], nucleation of the inner core [11,12], and the influence of the geomagnetic field on the atmosphere and creating conditions suitable for the evolution of life [13], among others.

In contrast to the complexity of scientific problems to which it has been applied, the form of the Arrhenius-Néel law is extremely simple,

$$\tau = \tau_0 \exp\left(\frac{E_B V}{k_B T}\right) = \frac{1}{f_0} \exp\left(\frac{E_B V}{k_B T}\right), \quad (1)$$

where τ is the mean time a system stays in a local energy minima magnetic state (with energy E_1) before it rotates to a second state (with energy E_2) or vice versa. τ_0 is the characteristic switching time of a magnetic nanostructure and its inverse $f_0 = 1/\tau_0$ the attempt frequency of the system. The relaxation time τ depends on the ratio of the energy barrier $E_B V$ between the local energy minima states and the thermal energy $k_B T$ of the system. k_B is the Boltzmann constant and T is the absolute temperature of the system. In nanomagnetism, E_B is determined by the different types of anisotropies in the system, e.g., magnetocrystalline or shape anisotropy [14]. In the particular case of isotropic magnetite nanoparticles, cubic magnetocrystalline anisotropy determines the energy barrier as $E_B = K_C/12$, where K_C represents the negative cubic energy above the Verwey transition temperature.

Different methods exist to calculate the energy barrier E_B of a magnetic nanostructure such as the constrained Monte Carlo [15] or the nudged elastic band method [16–18] applied beyond the single-domain (SD) regime to larger vortex and multidomain magnetite particles [19]. In contrast, the determination of τ_0 is more complicated and a wide range of values exist in the literature, spanning from 10^{-7} to 10^{-13} s for the case of iron oxide nanoparticle systems [20–24]. The disparity in these values has important consequences for paleomagnetic recordings in the determination of whether a natural sample has kept its original magnetization. In magnetic hyperthermia τ_0 determines which nanoparticle size will optimize the specific absorption rate (SAR) [24]. For

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simplicity, an approximate value for the attempt frequency of 1 GHz has been widely assumed in the literature derived from the effects of magnetic relaxation in magnetic nanoparticles have on their Mössbauer spectrum [25], but this required highly characterized experimental samples and the fit to theory requires several simplifications. Additionally, two independent analytical expressions for τ_0 were reported in the literature by Néel [7] and Brown [26] that are both volume and temperature dependent. In practice f_0 is considered a constant and whether the volume or temperature play an important role on the value of τ_0 is still an open question.

In this work we numerically determine an accurate value for τ_0 of magnetite nanoparticles using atomistic spin dynamics which models the time evolution of the magnetization time in the presence of thermal fluctuations [27]. The value of τ_0 is calculated for magnetite nanoparticles of varying volumes, different temperatures, and for two different values of magnetocrystalline anisotropies.

II. METHODS

To model the dynamics of magnetite nanoparticles we use a Heisenberg spin Hamiltonian

$$\mathcal{H} = -\frac{1}{2} \sum_{i \neq j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{2} \sum_i k_c (S_{i,x}^4 + S_{i,y}^4 + S_{i,z}^4), \quad (2)$$

which considers the magnetic moments to be localized at the magnetic atoms [28]. $\mathbf{S}_i$ is a unit vector representing the direction of the magnetic moment of the atom at site i . J_{ij} is the exchange energy between the magnetic moments located at i and j , respectively, where exchange interactions are mediated by Fe-O-Fe superexchange bonds. k_c represents the cubic magnetocrystalline anisotropy energy experienced by the magnetic moment i . Exchange parametrization is taken from Ref. [29] where it was successfully used to describe the main bulk properties and anomalous magnetic phenomena in magnetite thin films in the presence of antiphase boundaries (APBs). For the magnetic anisotropy of magnetite we considered two different values in this work, $k_c = -1 \times 10^{-24}$ J/atom and $k_c = -1 \times 10^{-23}$ J/atom. The low-anisotropy case provides a 300 K value for the energy barrier close to that measured experimentally for bulk magnetite $K_C = -1.1 \times 10^4$ J/m³ [30] (see results). The high-anisotropy value is an upper bound for magnetite samples found in nature where imperfections can be a significant source of magnetic anisotropy.

The spin system's time evolution is governed by the atomistic Landau-Lifshitz-Gilbert (LLG) equation,

$$\frac{\partial \mathbf{S}_i}{\partial t} = -\frac{\gamma_i}{1 + \lambda_i^2} \mathbf{S}_i \times (\mathbf{B}_i + \lambda_i \mathbf{S}_i \times \mathbf{B}_i), \quad (3)$$

where $\gamma_i = 1.76 \times 10^{11}$ T⁻¹ s⁻¹ represents the gyromagnetic ratio, and $\lambda_i = 0.063$ denotes the Gilbert damping parameter. The damping constant value for magnetite is obtained from ferromagnetic resonance measurements [31]. The effective field $\mathbf{B}_i$ acting on spin i is derived from the Hamiltonian and is given by

$$\mathbf{B}_i = -\frac{1}{\mu_i} \frac{\partial \mathcal{H}}{\partial \mathbf{S}_i} + \boldsymbol{\zeta}_i, \quad (4)$$

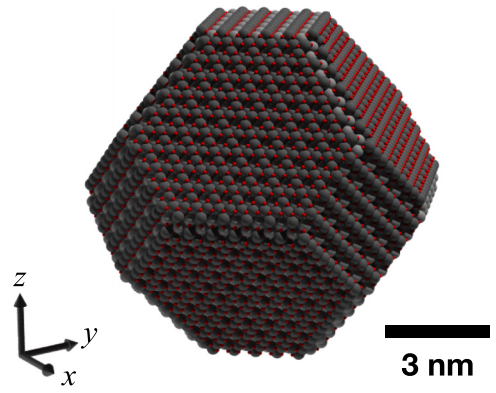


FIG. 1. Structure of a truncated octahedral faceted magnetite nanoparticle. Dark and light gray spheres represent the tetrahedral and octahedral Fe sublattices, respectively, while red spheres represent the oxygen atoms. The x , y , and z directions show the $\langle 100 \rangle$ directions with the $\langle 111 \rangle$ easy magnetocrystalline directions orthogonal to the hexagonal planes. This particle corresponds to a 9-nm-diameter particle and has $\sim 15\,000$ magnetic atoms.

where $\boldsymbol{\zeta}_i$ represents the thermal fluctuations acting on the spins. These fluctuations are modeled as a Gaussian-distributed random variable $\Gamma_i(t)$, as expressed in the following equation,

$$\boldsymbol{\zeta}_i = \Gamma_i(t) \sqrt{\frac{2\lambda_i k_B T}{\gamma_i \mu_i \Delta t}},$$

with $\Gamma_i(t)$ having unit variance, k_B denoting the Boltzmann constant, T representing the temperature, and $\Delta t = 1$ fs as the integration time step. The magnetic moments are $\mu_{\text{Fe}_A} = 5\mu_B$ and $\mu_{\text{Fe}_B} = 4.5\mu_B$ for tetrahedral and octahedral sites, respectively. The calculations have been performed using the VAMPIRE software package [28,32].

Here, we study truncated octahedral faceted nanoparticles, one of the most common morphologies found in natural samples and laboratory manufactured crystals [33–36]. A characteristic truncated octahedral nanoparticle is shown schematically in Fig. 1(a). The larger particle sizes considered approach the stable single-domain (SSD) regime [19,37], i.e., collective behavior of the magnetic moments is exchange dominated rather than magnetostatic. It is not computationally possible to simulate magnetite nanoparticles with sizes above the critical SD diameter ($D_C = 60\text{--}85$ nm) [38–40], beyond which vortex domain states dominate. We therefore do not include magnetostatic energy in our calculations. As in previous studies [19,41] we define the nanoparticle size as that of the equivalent spherical volume diameter (ESVD) D , which is then faceted to obtain octahedral particles. Therefore $D > D_{\text{faceted}}$, where D_{faceted} is the diameter of a sphere with the same volume as the faceted nanoparticle. We study particle diameters in the range $D = 8\text{--}30$ nm, and temperature ranges from 150 to 400 K. Each particle size and temperature has been simulated for a maximum of 1000 ns.

The dynamics of magnetic nanoparticles are highly dependent on the particle size and temperature. Characteristic dynamics of a $D = 16$ nm nanoparticle are shown in Figs. 2(a)–2(c) for different simulation temperatures. The

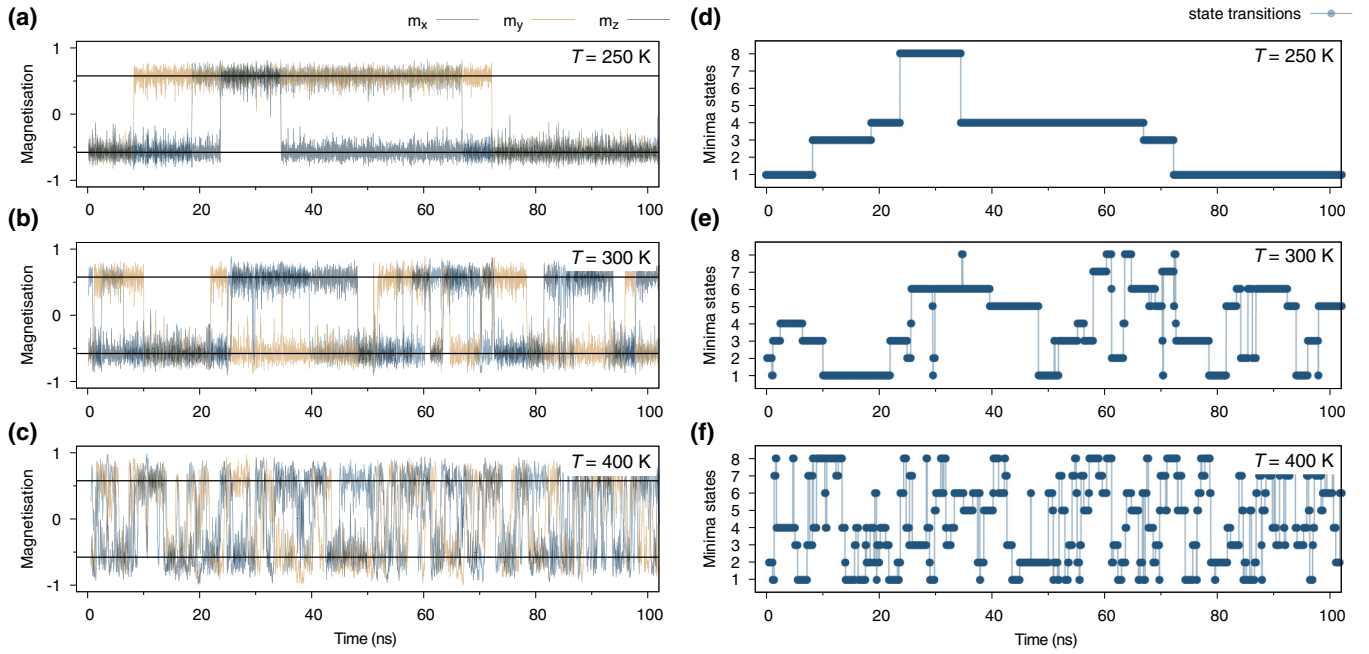


FIG. 2. Illustrative Langevin dynamics calculations of the time dependence of the magnetization for temperatures of (a) $T = 250$ K, (b) $T = 300$ K, and (c) $T = 400$ K for a fixed particle size ($D = 16$ nm). Different colored lines represent the Cartesian components of the normalized magnetization vs time and horizontal black dashed lines represent the minimum energy state directions for the negative cubic anisotropy energy. The magnetization exhibits telegraph noise where the magnetization is metastable in the minimum. The associated magnetic minimum is extracted from the time-dependent magnetization using the geofencing approach. The corresponding time evolution of each minimum state (labeled 1–8) for each temperature is shown in (d)–(f). This allows an accurate calculation of the relaxation time τ for all particle sizes and temperatures.

normalized components of the magnetization along the $\langle 111 \rangle$ directions, corresponding to the minimum energy states for the negative cubic magnetocrystalline anisotropy of magnetite, are shown by the horizontal dashed lines at $m_{x,y,z} = \pm\sqrt{3}/3$. Although calculated to 1000 ns, for clarity of the dynamics we only display the first 100 ns. The system exhibits telegraph noise as the magnetization is confined to occupy one of the eight energy minima for a certain period of time. For all temperatures, the fluctuations are rapid indicating superparamagnetic behavior on an experimental timescale. At $T = 250$ K [Fig. 2(d)] the magnetic anisotropy energy dominates the system such that the rate of magnetization switching from one equilibrium state to another occurs relatively infrequently within the 100 ns timescale. However, increasing the temperature by 50 K to room temperature (RT) and then by a further 100 K [Figs. 2(e) and 2(f)], the rate of magnetization switching increases by more than an order of magnitude for the same particle size. Increasing the particle volume for a given temperature produces the opposite effect as temperature does.

To accurately determine the attempt frequency it is first necessary to obtain a definitive value of the mean relaxation time τ . We use an alternative approach of geofencing, where the magnetization is associated with one of the eight local minima and is associated with that minimum until transitioning to a different minimum. The magnetization $\mathbf{m}$ is associated with a new minimum state α when $\mathbf{m} \cdot \mathbf{e}_\alpha > \beta$, where $\mathbf{e}_\alpha$ is the easy direction of the local minimum and β is the chosen threshold value. Each simulation is analyzed with different values of β , ranging from 0.90 to 0.95 in 0.01 steps.

For each simulation and β we determine the different transition times τ_i , where τ_i is the dwell time the magnetization remains in any given easy anisotropy axis. By collecting all τ_i obtained for each simulation (particle size and temperature) for all β we determine the average value of τ and its standard error. Figures 2(d) and 2(e) show the analysis done on the magnetization versus time simulations [Figs. 2(a)–2(c)] using $\beta = 0.91$. The first 2 ns of the simulations are always disregarded in the analysis for τ determination to allow the system to thermalize.

Collating all of the data for different nanoparticle sizes and temperatures we are able to determine the size and temperature dependence of the relaxation rate and extract τ_0 . The volume dependence of τ is displayed in Fig. 3(a) for the high-anisotropy case for various temperatures with a fit of the form

$$\ln\left(\frac{1}{\tau}\right) = \ln f = \ln f_0 - E_B \frac{V}{k_B T}, \quad (5)$$

where the intercept is the attempt frequency and the gradient gives the energy barrier. The low-anisotropy case is depicted in Fig. 3(b). For each temperature, τ exhibits a linearlike behavior with volume that has important implications. First, the linear nature of the data shows that the influence of the particle volume on the attempt frequency value τ_0 is negligible and its temperature dependence $\tau_0(T)$ can be determined from the intercept of a linear fit for each temperature. Second, the temperature dependence of the energy barrier E_B and magnetic anisotropy energy $K_C(T) = 12E_B(T)$ can be determined from the slope of the linear fit. The extracted values for the

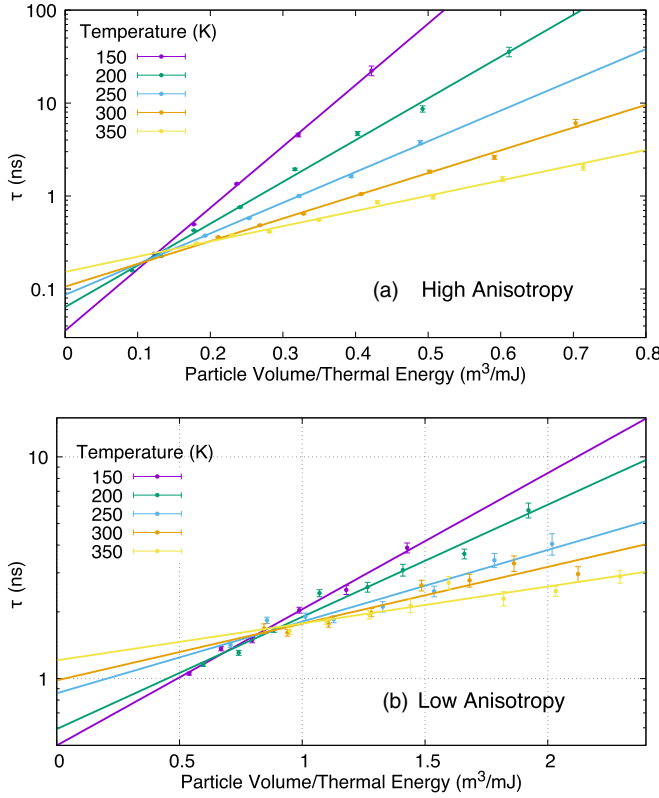


FIG. 3. Plot of mean transition rate obtained for each particle size for different temperatures. High and low anisotropy are depicted in (a) and (b). The intercept corresponds to the attempt frequency and the slope to the energy barrier.

temperature dependence of the attempt frequency $\tau_0(T)$ and the effective anisotropy energy are presented in Figs. 4(a) and 4(b), respectively.

The attempt frequency exhibits a temperature-dependent increase for both anisotropy values. In the low-anisotropy case, it follows a power law $\tau_0 \sim T^{1.1}$, with $\tau_0(300 \text{ K}) = 0.98 \pm 0.13 \text{ ns}$, remarkably close to the widely accepted value for magnetite. In contrast, for the high-anisotropy case, τ_0 increases more rapidly with temperature, approximately as $T^{1.6}$. Despite this temperature dependence, the variation in τ_0 remains modest, less than an order of magnitude difference across a 250 K temperature range. In both cases, the energy barrier (and hence the anisotropy) decreases monotonically with increasing temperature, in agreement with previous numerical studies on other materials [42]. For the low-anisotropy case, the calculated energy barrier at 300 K, $E_B(300 \text{ K})$, closely matches experimental values for magnetite anisotropy at room temperature [30]. This supports the suitability of our chosen zero-temperature atomistic anisotropy parameter, k_c , in reproducing magnetite's properties above the Verwey transition.

In this work we have simulated the dynamics of single-domain magnetite nanoparticles with cubic anisotropy in a range of sizes and temperatures using atomistic spin dynamics. The temperature range spans below and above room temperature, covering the most relevant cases for paleomagnetic and magnetic hyperthermia studies. We have studied the cases for low and high anisotropy representing fully pas-

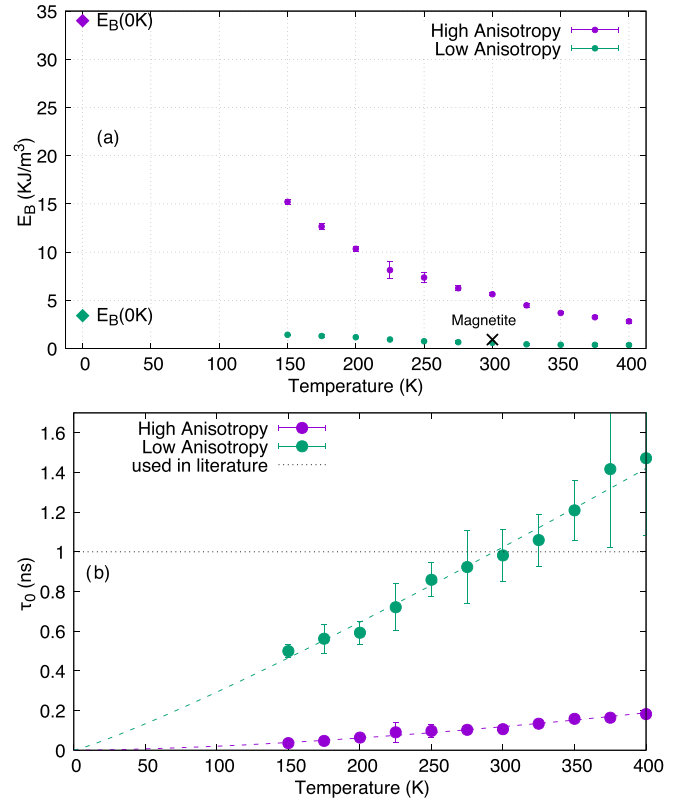


FIG. 4. Temperature dependence of the calculated (a) E_B and (b) τ_0 extracted from fits to Eq. (5). Dashed lines in (b) are fits to a $\tau_0 = a * T^b$ function. The error bars are extracted from the fit to the data. The cross in (a) represents the experimental value of the energy barrier at room temperature for magnetite [30]. The dotted line in (b) represented the widely assumed temperature dependence for τ_0 in the literature.

sivated Fe_3O_4 nanoparticles and particles with an enhanced anisotropy arising from either surface anisotropy or dopants such as Co. We find that τ_0 increases with temperature with a different rate depending on the anisotropy parametrization. The lower-anisotropy parametrization considered in this work, $k_c = -1 \times 10^{-24} \text{ J/atom}$, exhibits an energy barrier at room temperature very close to the experimental measured value for bulk magnetite as well as a value for $\tau_0(300 \text{ K})$, in very good agreement with the widely used one in the literature. Thus, the lower-anisotropy value is a reasonable value to reproduce bulk magnetite properties above the Verwey transition. The temperature dependences of τ_0 are approximately $\sim T$ and $\sim T\sqrt{T}$ for the low- and high-anisotropy cases, respectively. While τ_0 variation with temperature within the studied range is small (approximately one order of magnitude) we believe these results here provide an atomistic calculation of τ_0 , confirming experimentally determined values, and will provide additional accuracy in magnetic hyperthermia treatment design as well as estimates of paleomagnetic stabilities of recorded terrestrial and extraterrestrial samples.

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de Córdoba [44], which are part of SNCAD, República Argentina.

DATA AVAILABILITY

The data and code used in this study can be found in the Zenodo repository [45], which includes the code used for analyzing magnetization versus time as well as the data used to build this study.

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