

Premelting in dissolution of cemented carbides

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The dissolution behavior of tungsten carbide (WC) particles in liquid cobalt is investigated using *ab initio* and classical molecular-dynamics calculations. It turns out that at the atomic level there is a complex interplay between surface properties, bulk diffusion, and dissolution. It is found that carbon-rich shells form around dissolving WC particles, creating a semidissolved state. The dissolution process is decelerated by trapping carbon atoms via the formation of carbon-carbon bonds, both on the surface of dissolving particles and in the surrounding semidissolved shell. Upon reaching a critical particle radius, the dissolution rate sharply increases, driven by changes in the number of carbon-carbon bonds, resulting in a premelting behavior. The existence of a semidissolved shell and premelting behavior advance our understanding of dissolution mechanisms at the atomic scale and can be applicable for controlling dissolution processes that are an important part of coarsening of WC particles, a phenomenon taking place during cemented carbide manufacturing.

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I. INTRODUCTION

Metals of the groups VA and VIA (V, Nb, Ta, Cr, Mo, and W) form hexagonal carbides. Tungsten carbide (WC) favors a hexagonal crystal structure α WC (*hP*2, space group $P\bar{6}m2$) at room temperature [1] that remains stable up to 3049 K. A combination of strong ionic and covalent bonding together with metallic bonding is responsible for the extreme hardness and high melting point of WC [1,2]. At temperatures above 2789 K, substoichiometric WC can transform to a cubic WC_{1-x} with a rocksalt-type structure [3–5]. In the binary system, there is also a semicarbide phase W₂C that forms three polymorphs as a function of temperature. It should be mentioned that the substoichiometric carbide WC_{1-x} and the semicarbide W₂C melt at lower temperatures than the stoichiometric WC [6].

Invented casually in the search for a substitute for diamond drawing dies for the drawing of tungsten filaments in light bulbs by researchers at Osram laboratories [7,8], cemented carbides are composite materials made of carbide particles embedded into a binder metal. Titanium carbide (TiC), tantalum carbide (TaC), or tungsten carbide are among the most common carbides used as the aggregate. Tungsten carbide bonded by cobalt is a material of significant industrial and technological importance and is extensively used for cutting, milling, drilling, and turning tools applications [2]. Blending

together a unique combination of hardness and toughness inherited from the hard WC and softer (and more ductile) Co, cemented carbides are manufactured by sintering WC grains and soaking them in a liquid Co matrix [9]. During the soaking process, the average carbide grain size increases due to Ostwald ripening, where larger grains grow at the expense of small grains dissolving, resulting in an increase in the average grain size. Interdiffusion and interfacial properties govern this process and are considered in the classical analysis performed by Lifshits, Slyozov, and Wagner (LSW) [10,11]. Both studies show a homogeneous particle size distribution with an average size increasing with time. This homogeneous particle size distribution has been observed experimentally [12]. Computational studies on WC-Co interfaces have also been performed [13–15].

Abnormal grain growth occurs when large grains consume smaller grains, promoting the formation of an abnormally large grain. In cemented carbides, where the size of WC grains is distributed in the range of μm or less, abnormal grain growth can lead to grain sizes of several hundred μm [12,16,17]. The growth and/or dissolution behavior of WC particles in liquid Co has been studied through different experimental [18] and theoretical approaches [16]. Several previous studies have explored the dissolution of WC in liquids [19,20], including Co. Also, the dissolution of Co from WC-Co hard metal scrap was investigated experimentally by Kim *et al.* [21]. However a comprehensive understanding of the dissolution mechanism is still lacking.

In this study, we investigate the dissolution of WC in liquid Co at the atomic level, providing new insights into the dissolution behavior and underlying mechanisms. We employ classical molecular-dynamics calculations, using an interatomic potential based on an analytical bond-order scheme developed using experimental data and first-principles calculations [22,23], to study the atomic structure and dynamics at the WC(solid)–Co(liquid) interfaces during dissolution of WC

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in liquid Co. To better approximate the structure of real crystals, we create multiple WC particles with screw dislocations in the basal and prismatic planes. After embedding the WC particles into liquid Co, we observe dissolution and analyze the dissolution kinetics, as well as the structural atomic-scale changes that occur during the process. The findings shed light on the underlying mechanisms of the dissolution and provide insights into the factors that influence the dissolution behavior of WC in liquid Co.

II. METHODOLOGY

The core structure of screw dislocation defects in both the basal and prismatic plane orientation is obtained utilizing *ab initio* calculations using a plane-wave method [24] with projector augmented wave (PAW) type pseudopotentials [25,26] and a gradient-corrected density functional [27] as implemented in the VASP package [28]. A 448-site supercell [$25 \times 27 \times 40 \text{ \AA}^3$ consisting of a free particle ($15 \times 17 \times 30 \text{ \AA}^3$), surrounded by vacuum layers of $5 \text{ \AA}$ in the x, y and $10 \text{ \AA}$ in the z directions] with a $5 \times 5 \times 5$ Monkhorst-Pack k -point mesh was chosen for the studying the core structure with c in the y direction and a in the z direction. One screw dislocation was introduced into each unit cell oriented normal to the basal or prismatic plane ($10\bar{1}0$). A periodic boundary condition was applied in the z direction parallel to the screw dislocation line, while fixed boundary conditions were used in the x and y directions. For the Brillouin zone integration, the first order of the Methfessel-Paxton method [29] and a Fermi-type smearing method with a width of 0.043 eV were used. A cutoff energy of 500 eV was chosen in all calculations. The convergence criteria were set to be 10^{-6} eV for the total energy and $10^{-4} \text{ eV/\AA}$ for the forces, and the ionic positions were also allowed to relax in the direction parallel to the screw dislocation cores in all cases.

The molecular-dynamics (MD) simulations were performed using the Large-scale Atomic Molecular Massively Parallel Simulator (LAMMPS) package [30] to perform time integration of Nose-Hoover style equations of motion. The positions and velocities were sampled from the canonical (NVT) ensemble. First, we computed some thermodynamic properties of WC and Co substances through MD simulations to verify the performance of the analytical bond-order interatomic potential [22]. The interactions for the W–C system are those of Ref. [22], and the W–Co, C–Co, Co–Co interactions were fitted to describe WC–Co interfaces and configurations with dissolved W and C in Co [23] (details as provided in the Supplemental Material [31–36]). Supercells of WC and Co $70 \times 70 \times 70 \text{ \AA}^3$ containing $\sim 182\,000$ atoms were created and thermalized for 1 ns to the desired temperatures in the range $2200\text{--}2800 \text{ K}$, with an increment of 300 K , using a time step of 1 fs and an isothermal-isobaric ensemble (NPT). Subsequently, the system was thermally equilibrated using a Langevin-type thermostat for an additional 1 ns . After the initial thermalization of the system, the WC particles were created using the Atomsk package [37] and the WulffPack package in Python [38] with screw dislocation core structure obtained from *ab initio* calculations. We note in passing that the core structures obtained from *ab initio* calculations were similar to those obtained using the analytical bond-order

potential [22] with fitted parameters for the W–Co, C–Co, and Co–Co interactions [15] performing an energy minimization with periodic boundary conditions in the direction parallel to the screw dislocation line (z direction).

WC particles of three different shapes were created: one discoid consisting of $\sim 19\,000$ atoms, a sphere with $\sim 3\,000$ atoms, and a hexagonal prism with $\sim 5\,000$ atoms, with screw dislocations oriented in the basal and prismatic planes. Afterwards, the WC particles were embedded into the liquid Co. Subsequently, an additional MD run was carried out until the WC particles fully dissolved into the liquid Co.

To measure the dissolution rate and dimensions of the WC particles in real time, the Open Computer Vision Library OpenCV [39] and the Canny edge detection algorithm [40] were utilized. Snapshots of the dissolving particles were generated using the Open Visualization Tool Ovito [41], and subsequently grayscale images were produced and preprocessed to enhance contrast and reduce noise. This was achieved through Gaussian blurring [42], ensuring uniform intensity distribution and reducing high-frequency noise in the grayscale images. The edge detection process was then performed using the Canny edge detection algorithm [40,43].

Subsequently, a Sobel kernel is used to filter the smoothed image [44] in both horizontal and vertical directions to obtain the first derivative in the horizontal direction G_y and vertical direction G_x . From the two images, the edge gradient G and direction angle θ for each pixel were found as

$$G = \sqrt{G_x^2 + G_y^2}, \quad \theta = \tan^{-1} \left(\frac{G_y}{G_x} \right).$$

After obtaining the gradient magnitude G and direction angle θ , a full scan of the image is done to remove any unwanted pixels that may not belong to the edge. Two threshold values, min_{val} and max_{val} , are applied to the detected edges. Edges with intensity gradients more than max_{val} are accepted as edges, and those below min_{val} are considered to be nonedges, and therefore discarded. The threshold values for edge detection were empirically determined based on image contrast and feature sharpness, ensuring optimal edge delineation. To visualize the detected edges, the output binary images were overlaid on the original images and the edge was visualized via a yellow line. The dimensions were measured via analysis of the detected boundaries. The maximum length of a single C–C bond was set to $2.04 \text{ \AA}$. The C–C bonding properties were analyzed using ovito [41]. The C–C bonds lengths were calculated using vesta [45].

III. RESULTS AND DISCUSSION

To have a complete understanding of the dissolution, diffusion of all atomic species in liquid cobalt is studied and presented in the Supplemental Material in relation to benchmarking the performance of the interatomic potential [22,23]. The analysis shows that C has the fastest diffusion in liquid Co, followed by Co self-diffusion, while W as an oversized impurity has the slowest diffusion. Therefore, it is natural to expect that, upon WC dissolution into liquid Co, C will quickly diffuse out while leaving W behind. As will be shown below, there are more aspects of the dissolution process

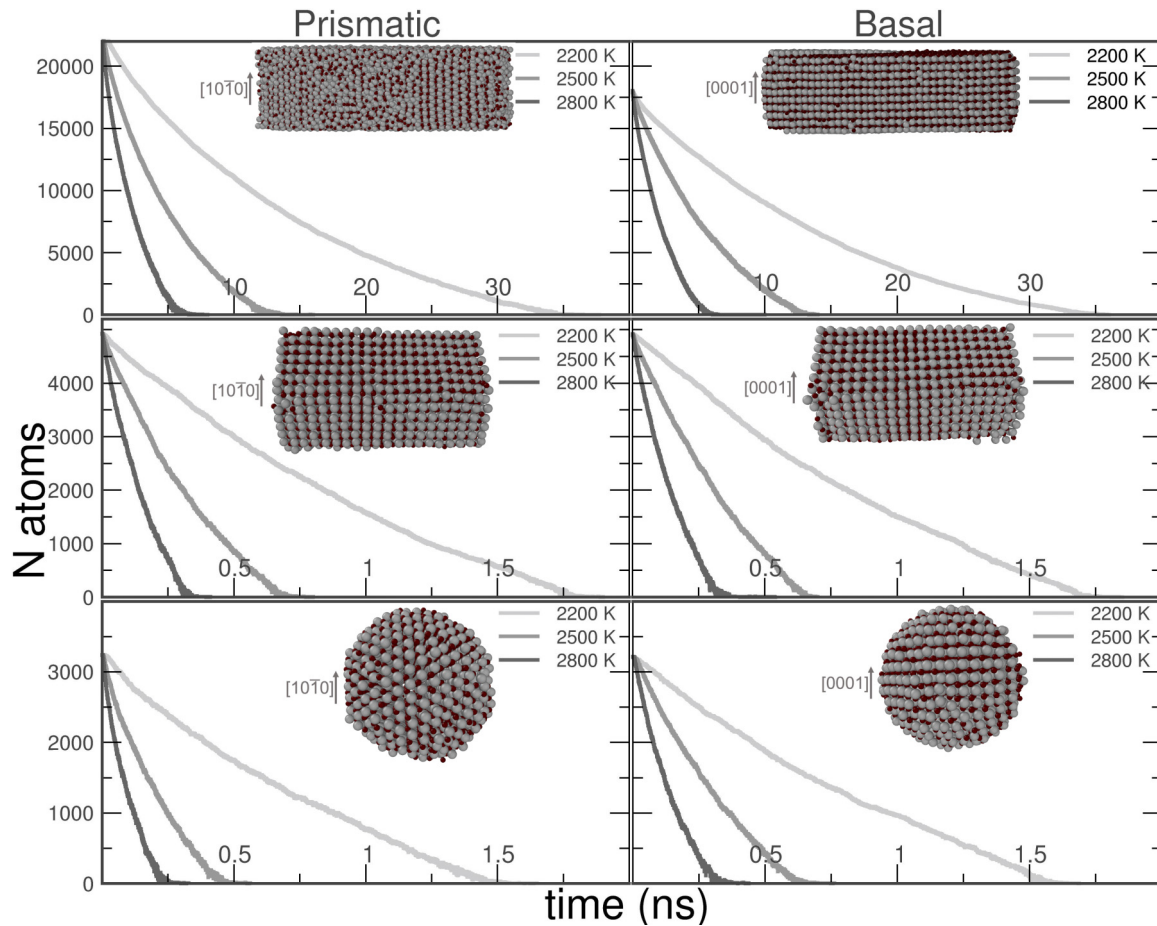


FIG. 1. Dissolution of tungsten carbide particles into liquid cobalt. The gray and brown spheres represent tungsten and carbon atoms, respectively. The orientation of the screw dislocation is shown with an arrow and the crystal direction index alongside each particle.

related to C. Furthermore, we perform the dissolution simulations for different initial particle geometries to observe the effect of particle shape and some universal features that are shape-independent.

The computational experiments conducted provide new data on the dissolution dynamics of WC particles in liquid cobalt, demonstrating that these dynamics are highly sensitive to particle size and geometry. Upon relaxation, the screw dislocations begin to dissipate, most likely due to the image stress they are subjected to, inducing a slight distortion in the particle shapes.

The composition of the WC-Co system is always carefully chosen such that the WC/Co ratio is less than 0.3% to ensure that the solubility limit is not exceeded even when the WC particle is fully dissolved in liquid Co. Initially, upon immersion in liquid cobalt, we observe the dissolution of all WC particles, as illustrated for various particle geometries with screw dislocations oriented in the prismatic and basal planes in Fig. 1. Furthermore, a significant increase in dissolution rate is observed when the dissolving particles become smaller than a critical radius, denoted as r_c (Fig. 2). The critical radius r_c is presented in Table I.

Here we report the longest dimension (height,width) of the dissolving WC particle at its critical size. One should keep in mind that the particles are dynamic during the dissolution and are not always perfectly spherical. This is more pronounced

in the case of discoid and hexagonal prism geometries where the particles are more ellipsoidal than spherical. In all cases, the largest axis of the ellipsoid is reported as the particle radius in Table I. For discoid and hexagonal prism geometries, this may correspond to either the height or the width of a dissolving particle, determined with precision of up to ± 2 Å. The particle dimensions at critical size for $T = 2500$ K are specified in Fig. 6. At this critical size, the dissolution process accelerates sharply, with both the height and width of the particles decreasing at a notably faster rate. This observation highlights the existence of a threshold beyond which dissolution becomes considerably more efficient, suggesting that particle size plays a key role in governing the overall dissolution kinetics in the system.

Another intriguing observation from the dissolution simulations is the formation of a WC-enriched shell around the dissolving particles, a phenomenon that occurs consistently regardless of the particle geometry, temperature, or linear defect orientation. This shell is formed around the dissolving particles and is detected by counting the W and C atoms that are at a distance greater than 2.906 Å from the surface of the WC particles. This shell is 14 ± 2 Å thick and remains stable until the particles dissolve beyond the critical radius r_c . The WC enriched shell is also characterized by carbon-carbon (C-C) bonds which appear to act as a temporary barrier impeding further dissolution (Fig. 3) by forming a semidissolved state.

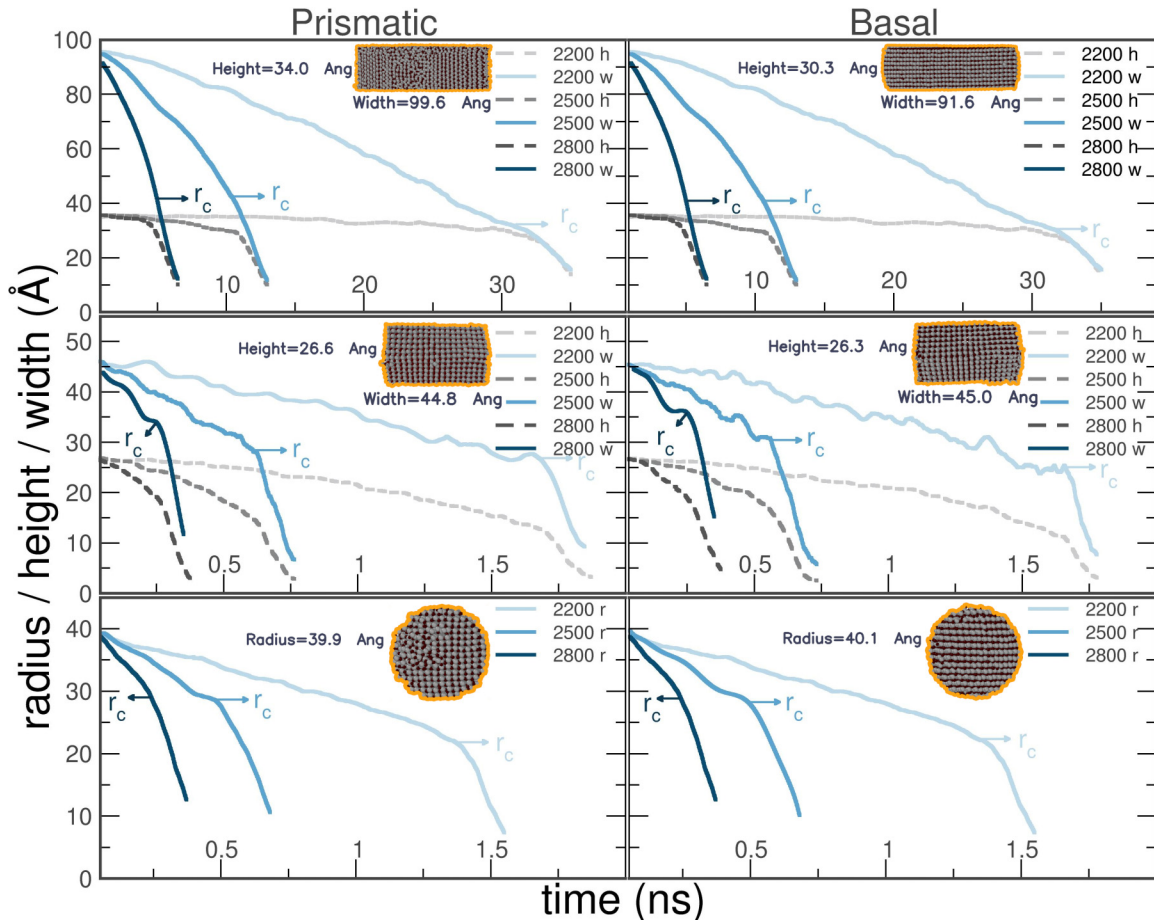


FIG. 2. Dimensions of tungsten carbide particles during dissolution into liquid cobalt as calculated using the OpenCV code library [39] and visualized with the yellow line surrounding the particle. In every panel legend, the numbers correspond to temperature in K, and the letters h , w , and r refer to height, width, and radius. Arrows labeled r_c indicate the critical radius. The gray and brown spheres represent tungsten and carbon atoms, respectively.

The number of the C–C bonds in the surrounding WC enriched shell tends to increase linearly up until the WC particles dissolve to reach the critical radius r_c .

C–C bonds appear in dimers and trimers formed during the dissolution simulations. The length of these C–C bonds is presented in Fig. 4. The C–C bond lengths range from 1.5 to 1.9 Å, with a maximum C–C bond length cutoff at 2.04 Å. We note that carbon atoms never occur at such short distances inside the WC solid particle; there the usual C–C distances are ~ 2.9 Å. Elemental analysis of the semidissolved shell reveals a high concentration of carbon, implying that carbon atoms from the dissolving WC particles are slowed down by being

trapped within the structure of the surrounding carbon-rich WC shell (Fig. 5).

This trapping mechanism suggests a possible explanation for the temporary stabilization of the semidissolved state. The WC shell persists to exist until the particles reach the critical radius r_c . Beyond the critical radius, the surrounding WC shell rapidly dissolves and dissolution is no longer constrained by the C–C bonds on the surface of the dissolving WC particles and surrounding shell. Subsequently, it is diffusion that becomes the rate-limiting process. This marks a shift in the dissolution mechanism, whereby surface phenomena give way to bulk transport processes as the particles diminish in size.

Previously it was found that C atoms tend to reconstruct and form C–C bonds inside metal atom vacancies in transition-metal carbides [46]. Recent experimental studies by Stasiak *et al.* show the presence of C–C bonded structures inside metal atom vacancies in high entropy carbide thin films [47] and more recently Lorentzon *et al.* have also confirmed the presence of reconstructed N structures in HfN thin films [48]. Here the emergence of C–C bonded structures, both on the particle surface and within the semidissolved shell, further underscores the complexity of the dissolution process. These C–C bonded structures form prior to complete dissolution and

TABLE I. Critical radius, $r_c \pm 2$ Å.

Particle shape	Dislocation	$T=2200$ K	$T=2500$ K	$T=2800$ K
Discoid	[0001]	34.32	42.12	43.35
Discoid	[10 $\bar{1}$ 0]	34.73	41.30	42.84
Hexagonal prism	[0001]	26.33	31.61	36.08
Hexagonal prism	[10 $\bar{1}$ 0]	28.32	30.04	35.15
Sphere	[0001]	22.88	27.86	29.96
Sphere	[10 $\bar{1}$ 0]	23.64	28.12	29.97

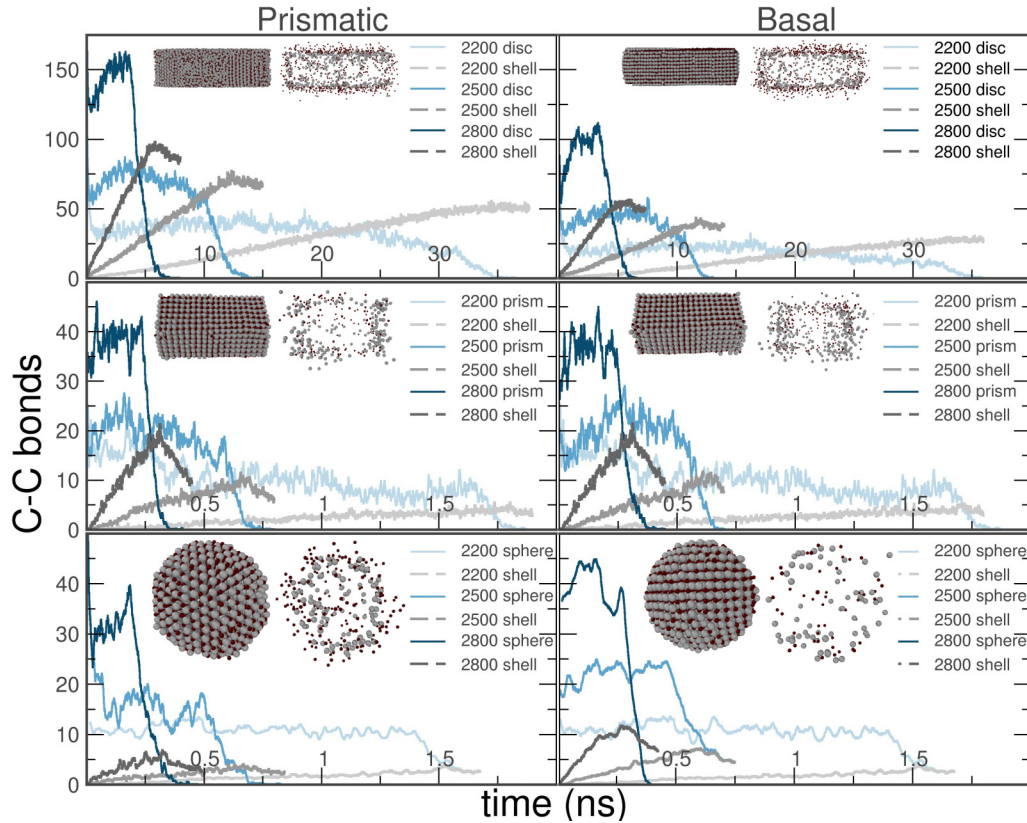


FIG. 3. Number of carbon-carbon bonds on the surface of tungsten carbide particles and in the surrounding shell during dissolution into liquid cobalt. The shell is defined as W and C atoms that are at a greater distance than 2.906 Å from the surface of the tungsten carbide particles. In every panel legend, the numbers correspond to temperature in K. The gray and brown spheres represent tungsten and carbon atoms, respectively.

mark a critical transition phase where surface chemistry and bulk diffusion become intertwined (Fig. 3).

Furthermore, the elemental analysis of the surrounding WC enriched shell shows that C is at a high atomic percentage at the initial stages of the formation of the surrounding shell. This implies that it is the C atoms that initiate the formation of the carbon-rich WC shell surrounding the dissolving particles (Fig. 5), and subsequently the C–C bonds contribute to the stability of the semidissolved shell surrounding the dissolving particles (Fig. 3).

The number of C–C bonds on the particle surface remains relatively stable during this stage, while those within the shell exhibit a linear increase as the particle approaches the critical radius r_c . Once this threshold is crossed, a rapid decrease in the number of C–C bonds is also observed, signifying a breakdown of the shell structure and a corresponding shift in the dissolution regime. The rapid decrease of the number of C–C bonds, consistently observed across all configurations, highlights a strong coupling between surface bonding interactions and the underlying diffusion dynamics driving the dissolution process.

Upon dissolving below the critical radius r_c , the particles exhibit a distinct premelting behavior, as evidenced by changes in the radial pair distribution function (Fig. 6). Premelting usually refers to a state where a thin layer on the surface of a solid transitions to a liquid state below the melting temperature of the solid [49,50]. Here we observe premelting

of the entire WC particles subsequent to dissolving beyond (below) the critical radius r_c . The radial pair distribution function shows that both carbon and tungsten atoms are progressively displaced from their lattice positions, signaling the onset of a transition from a solid to a liquid state.

A universal behavior is observed regarding the particle dimensions at r_c , the number of C–C bonds, premelting behavior, and dissolution rate throughout the dissolution process. In all our simulations, we see that the premelting behavior coincides with the particles reaching critical radius, and that rapid decrease in the number of C–C bonds both on the surface of the dissolving particle as well as in the carbon rich semidissolved WC shell surrounding the dissolving WC particles.

The consistency of the dissolution mechanism across particles of varying geometries and defect orientations underscores the robustness of the observed behavior. Despite differences in particle shape or defect structure, the dissolution process remains governed by the same underlying principles, suggesting that the interaction between WC and Co is largely driven by atomic-scale phenomena, particularly the behavior of C–C bonds and particle size observed in Figs. 2 and 3.

As the particles approach the critical radius, the reduction in C–C bonds correlates with the onset of melting, indicating a strong relationship between surface bonding and the phase transition. These findings suggest that once the number of C–C bonds falls below a critical threshold, the particles lose

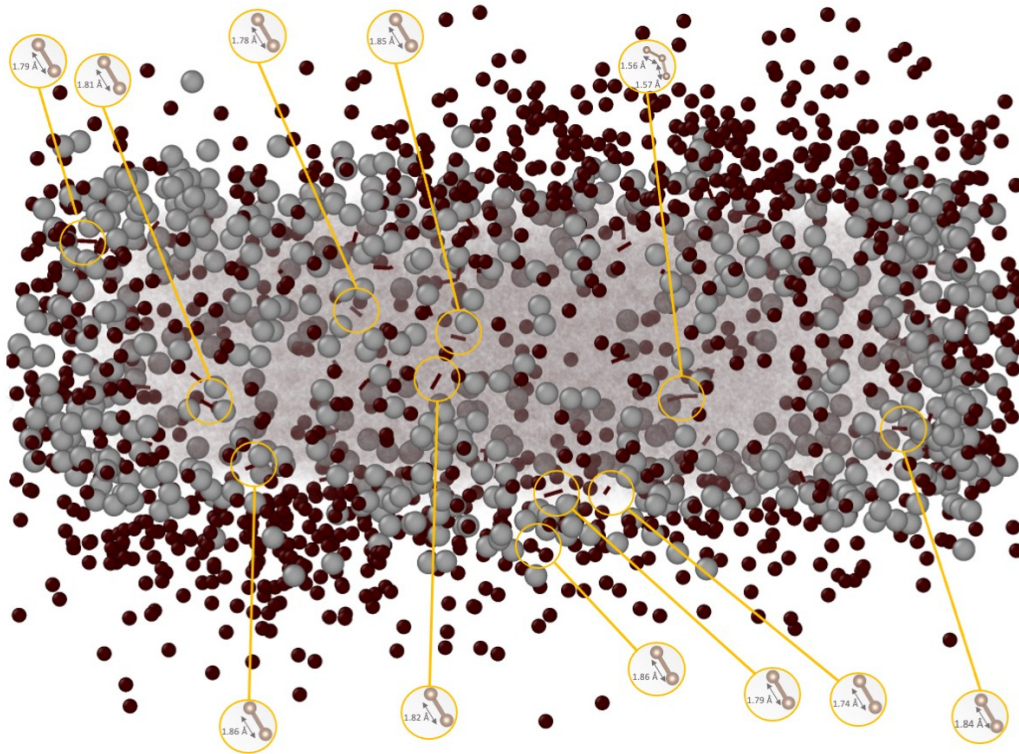


FIG. 4. Snapshot of dissolving discoid WC particle (with a screw dislocation oriented normal to the basal plane) at 2500 K and 1 ps. C–C bonds are displayed (dimers and trimers) with their respective bond lengths. The atoms inside the discoid WC particle are made transparent, only the W and C atoms in the shell are visualized. The shell is defined as W and C atoms that are at a greater distance than 2.906 Å from the surface of the tungsten carbide particles.

their structural integrity and transition into a liquid phase. This transition is likely facilitated by carbon trapping within the surface-bonded structures, which contributes to the observed phase change. The rapid dissolution and phase transition observed at the critical radius provide new insights into the atomic-level processes driving the dissolution of WC in liquid cobalt.

The analysis of atomistic simulation data reveals the intricate interplay between the number of C–C bonds on the surface and surrounding shell of the dissolving particle and the dissolution rate and diffusion into the liquid. When the number of carbon carbon bonds and the particle radius simultaneously drop below their critical values, the cluster is no longer solid and transforms to a liquid phase. The reported findings can serve to advance our fundamental understanding of dissolution mechanisms, which, in turn, is important for multiscale modeling of the WC particle coarsening process, of which the dissolution of small particles is an essential part.

IV. SUMMARY AND CONCLUSIONS

In this study, employing both *ab initio* and classical molecular-dynamics simulations, we investigate the dissolution behavior of tungsten carbide particles in liquid cobalt at the atomic level. The computations reveal several intriguing phenomena, such as accelerated dissolution of WC particles reaching a subcritical radius, premelting behavior, and the formation of carbon-carbon bonds on the surface of the particles as well as in the carbon-rich shells forming around dissolving

particles. The dissolution dynamics of tungsten carbide particles in liquid cobalt unveil a synchronous nature of the particle radius, the number of C–C bonds, premelting behavior, and dissolution rate, with possible implications for further understanding of interfaces at the atomic scale. Furthermore, the presence of carbon-carbon bonds contributes to the formation of a semidissolved WC state encapsulating the particles by a shell. This observation underscores the significance of considering both local surface phenomena and diffusion processes in particle dissolution. The investigation uncovers some universality in the dissolution behavior regarding particle geometry, the number of C–C bonds, premelting, and dissolution rate all coinciding simultaneously. This behavior is irrespective of the particles' initial geometry or defect orientation, emphasizing the complexity of the underlying dissolution mechanisms. Notably, the formation of carbon-carbon bonds on the surface of the particle and within the semidissolved shell around the dissolving particles emerges as a recurrent phenomenon. The elemental composition analysis of this shell reveals a significant carbon trapping, indicative of intricate surface interactions controlling the dissolution process. The reported findings provide atomically resolved information on the dissolution mechanisms at interfaces, and they offer insights for the design and optimization of materials.

Future investigations can shed light on the underlying mechanisms governing shell formation and carbon trapping phenomena in more detail. The findings presented here on dissolution kinetics of WC in liquid Co may have the potential for broader implications in materials science. These insights

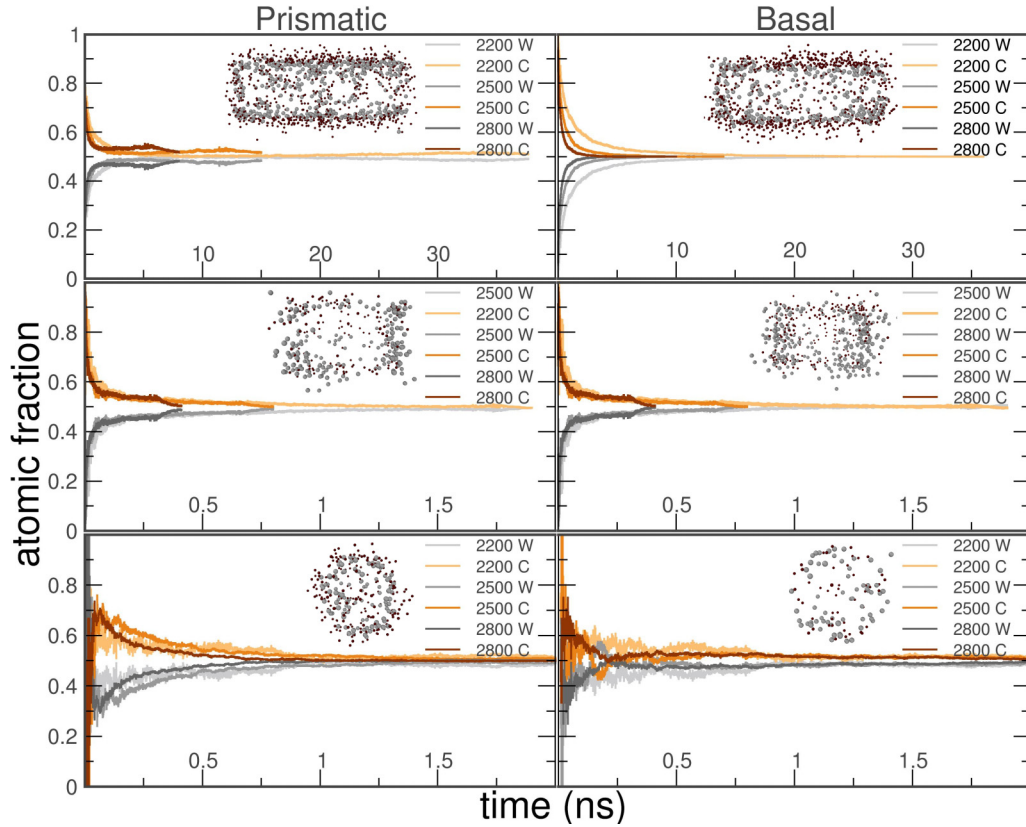


FIG. 5. Element content in shell surrounding the tungsten carbide particles dissolving into liquid cobalt. The shell is defined as W and C atoms that are at a greater distance than 2.906 Å from the surface of the tungsten carbide particles. The gray and brown spheres represent tungsten and carbon atoms, respectively.

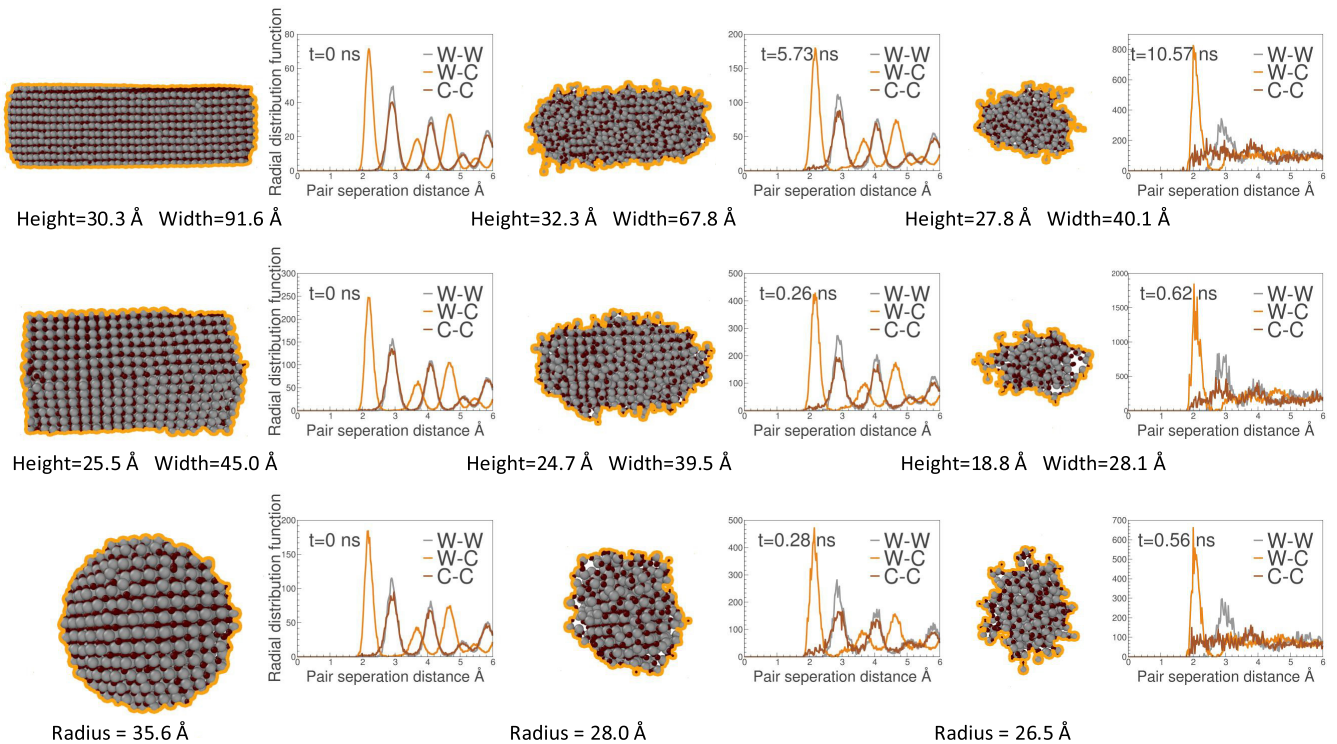


FIG. 6. Snapshots and radial pair distribution function of the tungsten carbide particles (with a screw dislocation oriented normal to the basal plane) dissolving into liquid cobalt at 2500 K. The gray and brown spheres represent tungsten and carbon atoms, respectively. The dimensions of the particles are calculated using the OpenCV code library [39] and visualized with the yellow line surrounding the particle.

could also be applicable for further understanding and controlling dissolution processes in manufacturing of cemented carbides.

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DATA AVAILABILITY

The data that support the findings of this article are available upon request from the corresponding author.

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