



# Molecular dynamics simulation study of the effect of temperature and grain size on the deformation behavior of polycrystalline cementite

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Received 1 August 2014; revised 21 September 2014; accepted 24 September 2014

Available online 22 October 2014

Molecular dynamics simulations combined with quantitative atomic displacement analyses were performed to study the deformation behaviors of polycrystalline cementite ( $\text{Fe}_3\text{C}$ ). At low temperature and large grain size, dislocation glide acts as the preferred deformation mechanism. Due to the limited number of slip systems at low temperature, polycrystalline cementite breaks by forming voids at grain boundaries upon tensile loading. When the temperature rises or the grain size reduces, grain boundary sliding becomes the primary mechanism and plastic deformation is accommodated effectively.

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**Keywords:** Polycrystalline cementite; Molecular dynamics simulation; Brittle-to-ductile transition; Grain boundary sliding

As a common second-phase constituent, cementite ( $\text{Fe}_3\text{C}$ ) plays an important role in determining the mechanical properties of steels [1,2]. Because cementite usually occurs in the form of fine lamellae or nanosized precipitates surrounded by ferrite matrix [3] neither its mechanical properties nor its deformation mechanism have been perfectly characterized, due to the difficulty of preparing pure bulk cementite specimens. Recently, bulk polycrystalline cementite with fine grains having sizes ranging from 0.5 to 3.2  $\mu\text{m}$  has been produced by mechanical milling and sintering [4–10]. At elevated temperature (>900 K), the sintered polycrystalline (SP) cementite shows superplastic deformation up to a few hundred per cent with steady-state flow stress and large strain without necking. In contrast, it shows brittle failure at ambient temperature, which can be recognized as a brittle-to-ductile transition (BDT) [4,9].

Umamoto et al. [4] reported that grain boundary (GB) sliding was a dominant deformation mechanism enabling superplastic deformation in SP cementite at elevated temperatures with few dislocation activities. Meanwhile, high density of dislocations with different Burgers vectors were formed in cementite single-crystal phase during high-temperature deformation of plain carbon steel [11]. The difference in these deformation mechanisms arises from the presence of GBs in SP cementite which usually do not exist

in the cementite phase embedded in steels. In addition, a change in grain size can affect the BDT temperature as well as the strength and ductility of SP cementite [4,10,12].

Although the bulk SP cementite experiments revealed intriguing properties, the measurements could have been affected by widespread impurities and pores produced during the prior processes of mechanical milling and sintering [12–14]. Microcracks, complicated metallic carbides and undesired ferrite are typically formed on the cementite GB site, and can affect the deformation of the cementite significantly. In other words, the observed behavior, such as the BDT, may not be an intrinsic property of polycrystalline cementite. If these non-intrinsic factors can be eliminated, it should be possible to understand the mechanism of SP cementite deformation more clearly.

Molecular dynamics (MD) simulations offer a unique opportunity to investigate the properties of materials with desired conditions at the nanoscale. In the case of cementite, molecular simulations based on ab initio methods or empirical potentials have been used to predict the formation energies of interstitial defects, growth morphology and the diffusion of carbon atoms [1,15–18]. However, less attention has been paid to the deformation mechanism of cementite. In this work, based on the MEAM Fe–C potential [19], we investigated the origin of the BDT and the mechanism of the superplasticity of polycrystalline cementite by studying the effect of temperature and grain size.

Two cubic nanocrystalline (NC) cementite samples containing 16 grains with random crystallographic orientation

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were generated by the Voronoi construction method [20,21] in order to create polycrystalline cementite. The edge lengths of each orthogonal sample were 19 and 30 nm to provide about  $6.5 \times 10^5$  and  $2.7 \times 10^6$  atoms and an average grain size of 9.7 and 16.4 nm, respectively. The MD simulations were carried out using the parallel MD code LAMMPS [22] with periodic boundary conditions in all dimensions at 100, 300, 700 and 1100 K. For each temperature, samples were relaxed for 200 ps under zero pressure with the Nosé–Hoover isobaric-isothermal (NPT) ensemble. Uniaxial tensile loading was applied to the maximum strain of 20%, with a constant strain rate of  $5 \times 10^8$  (s<sup>-1</sup>). The atomic shear strain distribution was calculated using the method of Shimizu et al. [23]. We applied a quantitative analysis to determine the contribution of dislocation glide and GB sliding, by calculating the changes in separation distances of atom pairs with regard to atoms belonging to the GB and the interior of the grain [24]. We also confirmed that there was no significant difference between simulations performed with different initial grain configurations of samples with the same grain size.

Figure 1 shows that the tensile stress increases with strain up to a certain peak stress and then gradually decreases, for all temperatures and grain sizes considered in this study. The peak stress is amplified due to the higher strain rate imposed in the MD simulation, and is significantly larger than the peak stress observed in experiments (0.3 GPa at 973 K [12]). The peak stress as well as the stiffness decreases as temperature increases, showing the thermal softening effect.

Our simulation results differ from the experiments, in which SP cementite broke abruptly via a brittle fracture without any plastic deformation. Furthermore, we found that the peak stress of samples of 16.4 nm grain size was larger than the peak stress of 9.7 nm samples for all temperatures, which is recognized as the inverse Hall–Petch effect. These differences occur because the grain size used in our simulation study was much smaller than that of experiments (0.7  $\mu$ m [12]) and large ductile deformation was accommodated via GB sliding.

An atomic strain analysis of deformed NC cementite was performed in order to understand the effect of GB and temperature on the deformation mechanism of this cementite [23]. The structures of initial and deformed NC cementite after 20% total tensile strain with grain sizes of 16.4 and 9.7 nm at temperatures of 100 and 1100 K are illustrated in Figure 2. We observed large shear strain along GBs for

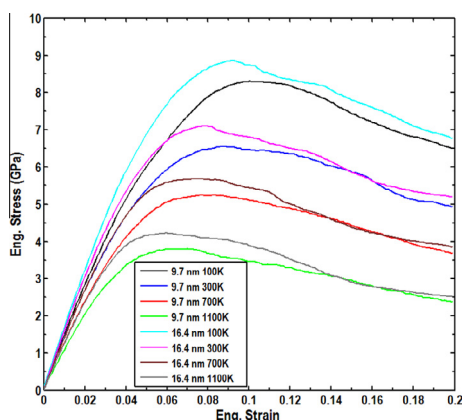


Fig. 1. Stress–strain plot for different grain sizes and temperatures.

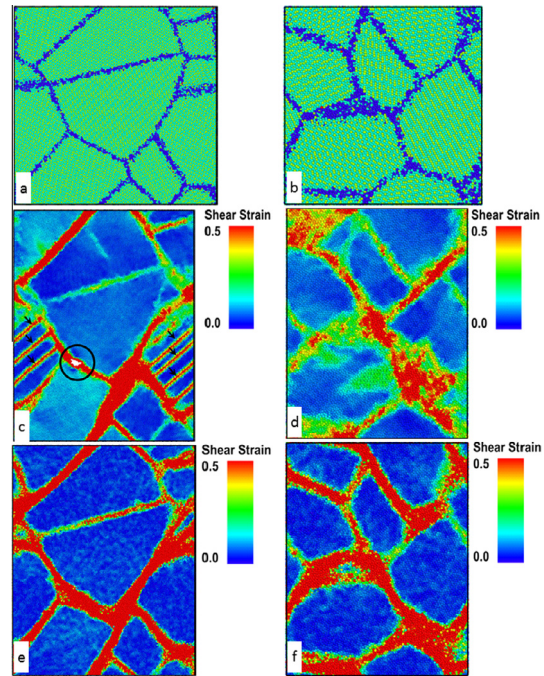


Fig. 2. (a and b) initial GB structure according to coordination number analysis of Fe atoms in the samples with average grain sizes of 16.4 nm (a) and 9.7 nm (b); blue atoms are in the GB structure. (c–f) Atomic shear strain distribution of Fe and C atoms after 20% total tensile deformation of NC cementite with (c) 16.4 and (d) 9.7 nm average grain sizes, at 100 K and with (e) 16.4 and (f) 9.7 nm average grain sizes at 1100 K. Red points indicate the atoms with a shear strain of  $> 0.5$ . Arrows show the formation of shear bands in (c) due to dislocation glide inside the grains. Void formation is also shown by the circle in (c). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

all simulation cells shown in Figure 2c–f, which explains the inverse Hall–Petch relationship seen in Figure 1.

We found two processes promoting plastic deformation: dislocation glide and GB sliding. Significant dislocation activities can only be found in Figure 2c, for the sample with large grain size at low temperatures. It is interesting to note that only a few grains possess intragranular shear bands from dislocation activity, while the other grains show shear strain only in the vicinity of GBs. The dislocations nucleate from the GBs due to the absence of an initial dislocation source inside the grains.

The straight slip traces reveal that the slip system in the cementite structure is simple and limited, since no cross-slip takes place. Cross-slip is hindered by the limited number of activated slip systems, such as  $[100](010)$ ,  $[001](010)$  and  $[001](100)$ , at low temperatures [11,25–27]. Thus, only a small fraction of suitably oriented grains having large Schmid factors can activate dislocation glide. Because of the small number of slip systems ( $< 5$  [28]), the sample does not accommodate large ductile deformation. This eventually leads to the accumulation of local stress which causes void formation at the GB, as shown in Figure 2c.

Our finding provides insight into the experiments in which SP cementite failed via brittle fracture with few dislocation activities at low temperature, and intragranular dislocation activity could only be seen in a small fraction of grains with suitable orientations [4,26]. Because the GB fraction was much smaller than in our simulations, the SP cementite in the experiments could not accommodate

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