Current Applied Physics 16 (2016) 1015–1025

Contents lists available at ScienceDirect

Current Applied Physics

journal homepage: www.elsevier.com/locate/cap

Nanoindentation study of cementite size and temperature effects in nanocomposite pearlite: A molecular dynamics simulation

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ARTICLE INFO

Article history:
Received 22 March 2016
Received in revised form
12 May 2016
Accepted 30 May 2016
Available online 31 May 2016

Keywords:
Nanoindentation
Molecular dynamics simulation
Nanocomposite pearlite
Cementite size effect
Dislocations blocking

ABSTRACT

We carry out molecular dynamics simulations of nanoindentation to investigate the effect of cementite size and temperature on the deformation behavior of nanocomposite pearlite composed of alternating ferrite and cementite layers. We find that, instead of the coherent transmission, dislocation propagates by forming a widespread plastic deformation in cementite layer. We also show that increasing temperature enhances the distribution of plastic strain in the ferrite layer, which reduces the stress acting on the cementite layer. Hence, thickening cementite layer or increasing temperature reduces the likelihood of dislocation propagation through the cementite layer. Our finding sheds a light on the mechanism of dislocation blocking by cementite layer in the pearlite.

1. Introduction

Pearlitic phase, a lamellar structure composed of alternating layers of ferrite and cementite, is a common constituent of steels and plays an important role in determining the mechanical properties of steels, such as toughness, strength and formability [1]. Compared to ferrite, pearlitic structure is known as a harder phase with higher strength due to the presence of cementite lamellae, and its mechanical properties are significantly affected by the cementite microstructure [2,3]. It has been found that the fine pearlite with small interlamellar spacing (~100 nm) and narrow cementite lamellae (~10 nm) shows higher ductility than coarse pearlite during plastic deformation [4–8]. Cementite layer act as a hard obstacle in front of ferrite dislocations and causes to dislocation pile up at the ferrite/cementite interface [9]. However, to the best of our knowledge, there has been no direct experimental or simulation study on the mechanism of the dislocation blockage by the cementite layer.

Nanoindentation is a mechanical test which uses an indenter with a known geometry to plunge into a specific site of the specimen by applying an increasing load [10]. It is widely used to determine the mechanical properties of thin films to clarify the effect of geometric confinement on mechanical properties [11]. In case of carbon steels, nanoindentation techniques have been applied to residual stress calculations in order to determine micro yield stress profile in surface layers [12,13]. Ohmura et al. performed a nanoindentation test on martensitic steel to directly measure matrix strength and separate it from grain boundary effect [14]. It can also be used to elucidate the cementite size effect on the deformation behavior of pearlite phase at nano scales, while complex equipment setup as well as the difficulty in preparing a sample with a desired cementite thickness makes the test costly and time-consuming. These difficulties can be circumvented by employing atomistic simulations.

Molecular dynamics (MD) simulations offer a unique opportunity to investigate the material properties with the desired conditions at nano scale. MD simulation has been widely used to virtually perform nanoindentation in order to investigate the elastic and plastic deformation mechanisms [15–18]. According to Chang et al. [19], the interlayer graphene thickness can affect the mechanical properties of nickel-graphene nanocomposite as well as indentation depth for dislocation nucleation. Goel et al. [20] have used MD simulations of nanoindentation to compare mechanical properties of Fe_3C (cementite) and Fe_4C iron carbides.

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http://dx.doi.org/10.1016/j.cap.2016.05.024
1567-1739/

In this study, we perform a series of nanoindentation tests of ferrite-cementite nanocomposites using MD simulations to investigate the role of cementite in blocking dislocation propagation in pearlite structure at various temperatures. For this reason, atomistic models of single crystal ferrite (Fe) film and ferrite-cementite nanocomposite thin films with different cementite thickness are constructed, and subjected to nanoindentation tests with different indenter radii at various temperatures. Our results show that increasing cementite thickness or increasing temperature makes dislocation penetration through the cementite layer harder to occur.

2. Simulation methods

Four ferrite-cementite nanocomposite samples with different thickness of cementite ($P = 0$, 1, 3, and 5 layers of cementite unit cells in the x–z plane) were prepared as depicted in Fig. 1 to investigate the cementite size effect (the thickness of cementite layer along $[010]_c$) and the temperature effect on the deformation behavior of pearlite under indentation. We chose $[111]_f \| [100]_c$, $[\bar{1}10]_f \| [001]_c$ and $(11\bar{2})_f \| (010)_c$ for the interface orientation relationship between ferrite and cementite according to Bagaryatsky [21] (with regard to cementite lattice constants $a = 5.05$ Å, $b = 6.69$ Å and $c = 4.49$ Å). Sample dimensions of pure Fe are 15 nm by 15 nm in the x–z plane and 8 nm in the y axis. The thickness of Fe layers is kept constant as 4 nm in pearlite samples, while the thickness of cementite layer is varied as 0.67, 2.0 and 3.35 nm in P1, P3 and P5 samples, respectively. The samples of P0 (pure Fe), P1, P3 and P5 were composed of *165,000*, *180,000*, *211,000* and *242,000* atoms, respectively. Ferrite and cementite have different lattice structures and lattice constants. The lattice misfit strain in Eq. (1) is relatively large for x and z directions (2.4% and 11.4%, respectively). In order to reduce the in-plane misfit strain in Eq. (2) in x–z plane, the samples were constructed with 30 by 37 ferrite unit cells and 29 by 33 cementite unit cells along x and z directions, respectively. Resultantly, the 0.4% and 0.25% in-plane misfit strains were imposed at the ferrite/cementite interface along x and z directions, respectively.

$$\Delta_{lattice} = \frac{d_{cementite} - d_{ferrite}}{d_{ferrite}}, \quad d : lattice\ constatnt \tag{1}$$

$$\Delta_{in-plane} = \frac{L_{cementite} - L_{ferrite}}{L_{ferrite}}, \quad L : cell\ dimention \tag{2}$$

The interatomic potential of Fe–C developed by Liyanage et al. [22], based on a modified embedded atom method (MEAM), was used to describe interatomic forces. This potential is fitted to structural, elastic and thermal properties of cementite at a wide range of temperature as well as the surface formation energy, polycrystalline elastic moduli and specific heat obtained from first-principles calculations and experiments [22]. Also, we found that generalized stacking fault energy curves obtained from the MEAM potential are consistent with those obtained from *ab initio* calculations, as presented in Appendix A. We also have used the potential to investigate the origin of brittle-to-ductile transition of nano-crystalline cementite [23]. The MD simulations were carried out using a parallel MD code, LAMMPS [24] with periodic boundary conditions in x and z dimensions at 100, 300 and 700 K. For each temperature, samples were relaxed for 100 ps under zero pressure with Nose-Hoover isobaric-isothermal (NPT) ensemble. All samples were indented with a constant velocity of 10 m/s along y direction by frictionless spherical indenter. We used three different indenter radii ($R = 3$ nm, 5 nm and 7 nm) in order to investigated the effect of indenter radius on the dislocation propagation through the cementite layer. The force on each atom was calculated by:

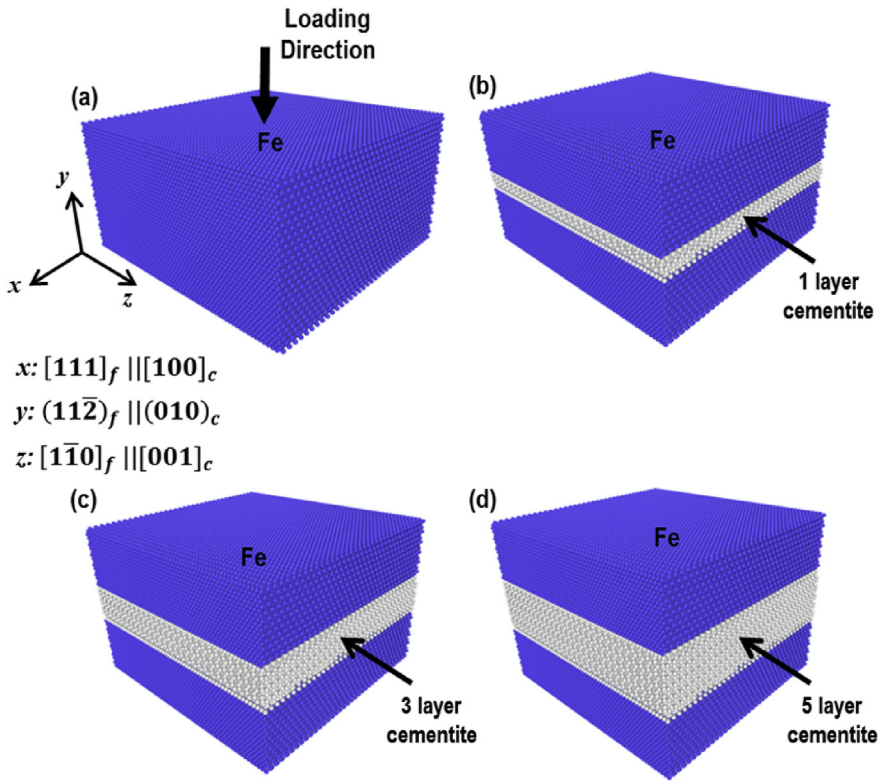

Fig. 1. Illustration of pearlite nanocomposite samples; (a) pure Fe, (b) P1, (c) P3 and (d) P5 samples. The position of cementite layers have been pointed by the back arrows.