Atomistic Simulation of Heavily Plastic Deformation of Pearlitic Steel: Nano-sized Processes of Wiredrawing and Indentation

K. Saitoh 1, K. Oda 2, K. Yoshida 2, M. Takuma 1, Y. Takahashi 1 and T. Sato 1

1 Department of Mechanical Engineering, Faculty of Engineering Science, Kansai University, 3-3-35 Yamate-cho, Suita, Osaka, 564-8680 Japan

2 Graduate School of Science and Engineering, Kansai University

E-mail: saitou@kansai-u.ac.jp

Abstract. We conduct molecular dynamics (MD) simulations of pearlitic steel in which iron and carbon atoms are included. The paper aims at clarifying micro- or nano-sized mechanism of plastic deformation of pearlitic steel in wiredrawing process. By using embedded atom method (EAM) potential, we construct a nano-sized computational wiredrawing model of pearlitic steel where lamellae structures of ferrite and cementite phases are attached to each other and it is subjected to conventional drawing condition using a hollow die. Basically, diffusion of carbon atoms around the ferrite-cementite interface is observed during plastic deformation. In order to recognize probable mechanisms by which carbon atoms migrate from cementite to ferrite, dislocation emission and its movement are observed in detail. Besides, the plasticity in pearlitic steel is also discussed in this research by using nano-indentation model where a nano-sized spherical indenter compresses lamellae structures of cementite and ferrite. Both wiredrawing and nano-indentation computational models provides new insight concerning atomistic mechanism occurring in heavily plastic deformation of pearlitic steel.

1 Introduction

Wiredrawing is a conventional plastic working method and has a long history, effectively producing a wide variety of engineering and metallic materials especially with wire, rod and pipe shapes. Recently, the demand for small-sized wire is more required in industry, so that the cutting-edge technique of making very thin wire is required and now it has come down to just several micrometers in diameter[1]. Though there have been developed a tremendously strong wire (fiber) from polymer material, the strongest wire-shaped material which has sufficient strength and reliability and fits to industrial use for infrastructure or transport equipment is still made of steel. Among them, pearlitic steel wire fabricated by wiredrawing technology is noteworthy and is recognized as the strongest one. The reason why the pearlitic steel is strong is believed that it has, in its microstructure, a combination of very thin fibrous structures where two different metallic phases, that is, ferrite ($\alpha$-Fe) and cementite ($Fe_3C$), become neatly aligned along the wire direction during drawing process. However, how those two phases become narrower and thinner retaining the thin lamellae shape during heavily plastic process like wiredrawing is not well understood so far. Experimentally, 3DAP (three-dimensional atom probe) technique or TEM (transmission electron microscopy) has been utilized to try to capture the change of those structures, but
dynamic arrangement of atoms or stoichiometric change, including phase transition and crystalline defects, induced by heavily plastic deformation during wiredrawing has not clearly perceived at all. Thus, atomistic simulation method is and will be playing an important role. For example, atomistic behavior of interface between ferrite and cementite can be simulated[2], and an assessment of working principle as for producing for nanometer-sized wiredrawing and materials’ flow are investigated[3]. There have been some researches for atomistic modelling of pearlitic steel[4][5], but the heavily plastic deformation like wiredrawing has not been fully investigated. The topic of the research is the effect of interface geometry (mutual relationship of crystalline orientation between cementite and ferrite) and energy on dislocation behaviour as well as diffusivity of carbon atoms. The corresponding experiment should be nano-indentation[6], in which very small indenter is pressed into the surface of specimen and any plastic deformation as well as elastic response there is observed from obtained force-depth curve. In this study, computational model of pearlitic steel is investigated by using precise EAM potential and molecular dynamics (MD) method along above context. Heavily plastic deformation of pearlitic steel are configured by modelling a conventional wiredrawing condition and more basic testing setup of nano-indentation. Nano-indentation model will be capable of investigating atomic behavior of crystalline defects during plastic deformation more in detail.

2 Theory and method

2.1 Potential functions for ferrite and cementite phases (for iron and carbon atomic system)

In this study, EAM (embedded atom method) potential for iron(Fe) and carbon(C) atomic system, in which many-body interaction between neighbor atoms is incorporated as well as primitive pair-wise interaction, is used[7]. There should be some possible choices in EAM potentials’ family (including modified EAM) for Fe-C system[8]. Among them, different two formulations of EAM potential are adopted for the present wiredrawing and nano-indentation models, respectively, here. It means that direct and quantitative comparison is difficult between two MD results, but it is certainly realistic that each results are reliable and precise. The EAM potential is generally formulated as:

\[ \Phi = \sum_{i=1}^{N} \left\{ F(\rho_i) + \sum_{j>i}^{N} V(r_{ij}) \right\}, \]

where \( \Phi \) is total potential energy of the system, \( F(\cdot) \) is called embedded energy function, \( \rho_i \) is electron density on the site of \( i \)-atom, \( V(\cdot) \) is a function of pairwise interaction and \( r_{ij} \) is distance between \( i \)- and \( j \)-atoms. Here, we use two EAM potentials. One is obtained by Ruda et al.(Ruda-EAM)[9] and it is constructed from well-known Mendelev II (EAM) potential which is just for Fe-Fe interaction. It is reformulated to become also including C-C and Fe-C interactions. The characteristic of Ruda-EAM potential is that a certain degree of condensation of carbon atoms often into cluster form is reproducible. Another one is proposed by Hepburn et al.(Hepburn-EAM)[10]. Technically speaking, Hepburn-EAM potential is already integrated into LAMMPS software[11] we are using. It is based on a first principle \textit{(ab initio)} calculation. The details of expressions of these two EAM potentials are omitted here.

2.2 Molecular dynamics modelling of pearlitic steel under heavily plastic deformation

2.2.1 Modelling of Pearlitic steel. Pearlite structure existing in carbon steel is composed of two crystal phases, ferrite and cementite, each of which are often called \( \alpha \) and \( \theta \) phases, respectively. The former has the body-centred cubic (bcc) lattice unit, and the latter has the orthorhombic crystal lattice unit. The interface between \( \alpha \) and \( \theta \) phases is not fully determined to any unique relationship. By theoretical consideration of crystalline matching based on experimental facts, there has been found three principal relationships between two crystal parts, namely, Bagaratsky(BA), Isaichev(IS) and Pitch-Petch(PP) relations as shown in figure 1. In this study, those three relations are compared. As for the nano-indentation model, at first, BA interface relation is scrutinized in this paper. The lattice constants for \( \alpha \) and \( \theta \) phases are checked by NPT-ensemble MD at 300 K with fully periodic lattice. \( a_\alpha = 0.286 \text{ nm} \) (one for ferrite: \( \alpha \)) and \( a_\theta = 0.437 \text{ nm} \), \( b_\theta = 0.514 \text{ nm} \) and \( c_\theta = 0.650 \text{ nm} \) (three for cementite: \( \theta \)) are obtained and those values are used in arranging cementite in pearlite models.
2.2.2 Computation model for wiredrawing process. This model assumes drawing process of nano-sized pearlitic steel wires. As shown in figure 2, the wire material is pushed through a hollow die with conical shape, by moving two edge regions with velocity constraint. The shape of die is designed as to mimic an actual large-sized conventional drawing die, which furnishes die-semi-angle of 7.0 degrees. The wire part has 7~8 nm in diameter. Since the atoms in the interface region across wire and die parts mutually exerts too strong interaction (attractive) force in non-treated setup, it is found that a certain relief of interatomic interaction has to be applied there so that the wire is smoothly drawn through the die hole. Calculation conditions of this drawing model are summarised in table 1. Interface plane between α and θ phases is placed in parallel to the drawing direction. The potential function for this model is Ruda-EAM[9].

![Figure 2. Molecular dynamics(MD) model for nano-sized wiredrawing of pearlitic steel.](image)

| property       | unit   | value(s)                  |
|----------------|--------|---------------------------|
| Cell size in x, y, and z directions | nm     | 9.8796, 9.8796, 16.7592   |
| Inlet diameter $D_{in}$ | nm     | 6.8796                  |
| Length of die land $L_0$ | nm     | 4.12                    |
| Die semi-angle $\beta$ | deg.  | 6.0                     |
| Moving velocity $V_{in}, V_{out}$ | m/s   | 38.3, 50.0             |
| Time increment $\times$ steps | fs    | $2.0 \times 20000$      |

2.2.3 Computation model for Nano-indentation process. For the purpose of investigating heavily plastic deformation around α-θ interface, a computation model of nano-indentation testing is configured. The nano-indentation experiment is well known as an actual nano-sized material testing method to see hardness or plasticity process, in particular, for thin film state by using very hard indenter. In this study, α and θ phases with very narrow thickness are stacked as shown in figure 3 and are pushed from one
side by a spherical indenter. Naturally, we will be comparing different directions of indenter push, but one arrangement in which landing of indenter takes place on the surface of α phase should become the most critical condition, because many dislocations will be emitted and be contained with relative ease inside the α part. The point of mechanisms is that how dislocations are transferred from α to θ, dragging carbon atoms around their interface. Computation conditions of this nano-indentation model is shown in table 2. The thickness of each lamellae structures should be several nm in this model, which is inevitable due to the limitation of computation size. The discussion on size effect of lamellae structure in pearlite is still open and is left to further studies, but the present model provides us important insight when nano-sized lamellae exists in the pearlite. Potential function for this model is Hepburn-EAM[10].

Table 2. Computation condition of nano-indentation testing performed by MD.

| property                        | unit | value(s) |
|---------------------------------|------|----------|
| The number of atoms             | -    | 141120   |
| Sizes l, h, b                   | nm   | 7.34, 12.47, 16.06 |
| Type of α / θ interface         |      | Bagaryatsky(BA): (001)₀ // (112)₀ |
| Indenter diameter D             | nm   | 10.0     |
| Pushing speed Vₚ                 | m/s  | 200.0    |
| Temperature                     | K    | 300      |
| Time increment × steps          | fs   | 1.0 × 100000 |

2.3 Dislocation mechanism and its detection method
In MD simulation, from perpetual output of position and velocity of atoms, many analyses can be conducted. Analysis of lattice defects is important to understand plasticity occurring inside MD cell. Recently, DXA method (Dislocation eXtraction Algorithm) is developed by researchers and the dynamic behavior of dislocations in crystalline lattice are successfully obtained from MD results[12]. (The DXA analysis operation is already integrated into visualization software called “Ovito”[13]).

3 Results and discussions
3.1 Behaviour of pearlite in wiredrawing process model
Figure 4 shows an example of wiredrawing model of pearlrite material. As the wire is drawn and its atoms go through the die, the α phase easily exhibits plastic deformation but the θ phase gets including some carbon clusters. This mechanism is understood as a kind of phase separation toward binary phase coexisting monoatomic C and Fe regions. The diameter of carbon atomic cluster approximately has grown until 1.5~2 nm. The reason why stoichiometric Fe₃C phase exhibits such phase separation is that Ruda-EAM potential function used in this wiredrawing MD model has energetically more stable state for C-C bonding than that for the initial Fe-C bonding. This behavior does not confirmed when using only pairwise interaction, which means that the nature of EAM potential function is responsible for.
These MD results predict that experimentally a segregation process of carbons will be induced by heavily plastic deformation.

**Figure 4.** Results of dislocation analysis (by DXA method[12][13]) and observed condensation of carbon atoms, comparing three different crystalline orientations of the interface in pearlite.

### 3.2 Behaviour of pearlite in nano-indentation process model

Figure 5 shows the results obtained by nano-indentation process model. In figure 5(a), the relation between force acting on the indenter in the pushing direction and the depth of indentation. In the first part of the curve, it exhibits a quadratic elastic response. After then, it shows several local drops of force value, which mean accumulation of plastic deformation. Figure 5(b)–(d) show dislocation behavior mainly in α phase. In this simulation, the indenter enters in the specimen from the side of α phase which is displayed in upper part in the figure. In fact, after structural relaxation process to adjust atomistic strain occurring around the α-θ interface, a kind of lattice defects called “misfit dislocations” emerges. As shown in figure 5(b), these dislocations seem relatively immobile because of conserving nature of Burgers vectors. Then, as shown in figure 5(c), indenter digs into α phase and soon dislocations are emitted from the contact area of indenter. It is observed that these dislocations overhang from the surface, forming almost dislocation loops. However, as shown in figure 5(d), those overhanging dislocations must interact with the α-θ interface and a part of them is likely to be adsorbed into θ phase. It is understood that this adsorption behavior tends to occur due to the very narrow width of α phase. Note that dislocations produced by indentation also interact with misfit dislocations left in MD cell and their interaction often lead to perfectly immobile dislocation. Unfortunately, dislocations in θ phase is not clearly defined, so they are not detected at this point. The detection method are expected to be developed in future studies.

### 4 Conclusion

In order to understand atomistic behaviour in wiredrawing of pearlitic steel, molecular dynamics simulation of nano-sized wiredrawing and nano-indentation are performed. Since precise EAM potentials are used, realistic behavior of atoms and lattice defects are obtained. For wiredrawing model, a possibility of condensation of carbon atoms up to about 2 nm in cluster size are discovered. It depends on the formulation of EAM potential. For nano-indentation model, emission of dislocations induced by indentation are reproduced. Interaction mechanism between emitted dislocations and misfit dislocation is successfully observed. Unfortunately, dislocation in cementite phase is not detected due to under investigation, but some dislocations in the ferrite phase emitted by indenter are probably absorbed inside the cementite phase.

**Acknowledgement**

This work was supported by JSPS KAKENHI Grant Number JP16K05994(Grant-in-Aid for Scientific Research (C)) and Nippon Steel & Sumitomo Metal Corporation. The authors would like to acknowledge those supports here.
Figure 5. Results of pearlite nano-indentation process model: (a) force-depth curve obtained during indentation process; (b), (c) and (d) visualized dislocations and carbon atoms remaining in the cementite phase (dislocation lines are detected by the DXA method [12] [13]).

References

[1] Zelin M 2002 Microstructure evolution in pearlitic steels during wire drawing Acta Mater. 50 4431-47
[2] Levchenko E V, Evteev A V, Belova I V and Murch G E 2009 Molecular dynamics simulation and theoretical analysis of carbon diffusion in cementite Acta Mater. 57 846-53
[3] Saitoh K, Sameshima Y and Daira S 2014 Nano-scale modelling and simulation of metal wire drawing by using molecular dynamics method World J. Nano Sci. Eng. 2 46498
[4] Guziewski M, Coleman S P and Weinberger C R 2018 Atomistic investigation into the mechanical properties of the ferrite-cementite interface: The Bagaryatskii orientation Acta Mater. 144 656-65
[5] Saitoh K, Yoshida K, Oda K, Sato T, Takuma M and Takahashi Y 2018 Molecular dynamics study on nano-sized wire drawing: possible atomistic process and application to pearlitic steel wire IOP Conf. Ser.: Mater. Sci. Eng. 307 012039
[6] Nix W D and Gao H 1998 Indentation size effects in crystalline materials: A law for strain gradient plasticity J. Mech. Phys. Solids 46, 411-25
[7] Daw M S and Baskes M I 1984 Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals Phys. Rev. B, 29, 6443-53
[8] Interatomic Potentials Repository (by NIST) https://www.ctcms.nist.gov/potentials/system/C-Fe/
[9] Ruda M, Farkas D and Garcia G 2009 Atomistic simulations in the Fe-C system Comp. Mater. Sci. 45 550-60
[10] Hepburn D J and Ackland G J 2008 Metallic-covalent interatomic potential for carbon in iron Phys. Rev. B 78 165115
[11] Plimpton S 1995 Fast parallel algorithms for short-range molecular dynamics J. Comp. Phys. 117 01-19
[12] Stukowski A and Albe K 2010 Dislocation detection algorithm for atomistic simulations Model. Simul. Mater. Sci. Eng. 18 025016
[13] Stukowski A 2010 Visualization and analysis of atomistic simulation data with OVITO - the Open Visualization Tool Model. Simul. Mater. Sci. Eng. 18 015012