Molecular dynamics study on nano-sized wiredrawing: possible atomistic process and application to pearlitic steel wire

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Abstract. The process of nano-sized wiredrawing is investigated by using molecular dynamics (MD) simulation in this study. The authors have constructed novel computation models of wiredrawing, in which a single wire of just a several nanometers in diameter is smoothly drawn through a perfectly rigid die together with lubrication mechanism and is forced to be shaped into thinner one. Interatomic potentials used in MD simulation is a conventional pairwise type useable for iron-carbon binary system (for pearlitic steel). For MD model of pearlite steel wire, it is recognized that ferrite-cementite interface effectively offers high-speed diffusion path for carbon atoms from cementite side to ferrite side (elementary mechanism of cementite decomposition). As conclusion, we showed by using atomistic simulation that nano-sized wiredrawing process is theoretically quite possible.

1. Introduction

Wiredrawing is a conventional plastic working technique in which a metallic wire (or bar, for larger diameter) is drawn through hard die and the diameter of material is effectively reduced [1]. In the drawing process, a wire is provided much strengthening as well as finer surface roughness. That is why the wiredrawing process has been used for manufacturing industrial equipment, such as suspension wire for a bridge, steel code for a tire and micro-sized wires for electric device. In recent years, demand for wire with smaller diameter is increasing and the finest wire manufactured in the industry has reached a few micrometers. This trend of wiredrawing technology will be ongoing, so nanometer-sized wire will be produced by drawing technique in near future. Compared with some other processing techniques to make nanowire (e.g. crystal growth techniques such as CVD, nano-metric physical process such as FIB, or nano-sized mechanical machining), drawing will be advantageous because it continuously reduces its diameter from normal size (millimeter or micrometer) to nanometer size. Besides, by drawing technique, microstructure inside of nanowire as well as surface state may be controllable.

However, there remains many problems in miniaturizing drawing process of normal size into nanometer size, such as atomistic friction between wire and die during processing. What is important and needed at this point is to theoretically assess possibility of drawing material in nano-sized scale. In this study, the authors are trying to model nano-sized drawing process by using atomistic simulation, i.e. molecular dynamics (MD) methodology. The MD method has predicted many unknown behaviors of nano-sized material, so it will fit this purpose [2].

On the other hand, from materials science's view point, it is crucial to understand the mechanism of strengthening during drawing. Usual strong wires are made of pearlitic steel, which is a compound between iron (Fe) and carbon (C) atoms. The pearlite phase is a key microstructure, but it has a complicated hierarchical structure in which cementite phase, a quasi-stable phase between Fe and C atoms, and ferrite phase, a pure α-Fe (body-centered cubic(bcc) structure) phase, are combined and aligned in lamellae arrangement [3]. The latest question of microscopic behavior of pearlite phase is how cementite decomposes by releasing carbons into ferrite and how such carbons affect the strength of the wire. This phenomena is often called "cementite decomposition". By using MD model, we will clarify this mechanism from an atomic point of view.

2. Theory and Method

2.1. Potential function for Fe-C system

In this study, as atomistic simulation methodology, molecular dynamics (MD) is used. In MD simulation, only initial atomic configuration and a potential energy function between atoms are specified, then trajectory and velocity of atoms time by time are obtained numerically.

The issue of determination of potential function is important. As of Fe-C system used here, the formulation by Levchenko *et al.* [4] is supposed to be better at this point since it is based on well-used Johnson-type potential for Fe-Fe interaction [5] and is including new *ab initio* data. By using this Fe-C potential function, the authors confirmed that a cementite crystal structure (Fe_3C) is well stably simulated. There have been a lot of elaborative works concerning formulating any precise potential function for Fe-C system or Fe_3C including EAM [6] or MEAM [7]. However, to our present knowledge, any reliable many-body potential function has yet appeared.

2.2. Nano-sized wiredrawing models, pearlite steel model and computation condition

In atomistic modelling of pearlite phase, we should consider microscopic portion of it, where a ferrite (α-Fe) phase having a highly symmetric unit and a cementite phase having the orthorhombic crystal unit are both arranged in narrow filament shape with only a few dozens of nanometres in width (it is often called "lamella" structure) [8][8]. The drawing is performed along the direction of these lamella filament. Due to the limitation of treatable numbers of atoms, the pearlite MD wire structure studied here is composed of one ferrite phase and one cementite phase.

The present MD model is set up as shown in figure 1. The wire has been inserted into a hollow die which has tapered shape in proportion to an industrial larger drawing die. In MD model, the die region comprises discrete atoms but they are totally constrained in space and the die behaves as rigid body block. Geometry of a conical drawing die is almost specified by die semi-angle and length of die land, and a resultant reduction ratio in cross-section area is an important factor.

In drawing, two chucking regions at both ends of the wire are forced to move with constant velocities which are in advance determined so as to maintain constant volume of the wire, supposing almost plastic deformation there [9]. The present wiredrawing is simulated with very high speed but it is not so unrealistic. However, there remains an issue due to miniature scale that friction between die and wire becomes enormously larger [10], regardless of wire speed. Therefore, in order to reduce friction at atomic contact, a kind of artificial lubricating mechanism has to be introduced in the present modeling. In the method, interatomic potential energy is multiplied by an arbitrary factor ω which is less than unity [2]. This affects directly pairwise potential so that cohesive energy, i.e. attractive force, near contact region is reduced by ω. As a result, friction coefficient μ between die and wire is effectively reduced to a smaller value such as μ=0.05 or lower.

In detecting dislocation or other lattice defects, we use a generic software for MD visualization and post-analysis called OVITO [11] along with DXA(dislocation extraction algorithm)[12]. By the DXA, dislocation lines are recognized together with information such as edge/screw type and size and direction of Burgers vector.

The important issue in constructing pearlite model is the relation of crystal orientation at the interface between ferrite (α phase: iron with very low carbon content) and cementite (θ phase: iron carbide) phases. We employ Bagaryatsky relation [13] which is supposed to exhibit relatively lower

lattice mismatch and lower interfacial energy between two crystal phases. The detailed arrangement is shown in figure 1(a). Several structural crystalline parameters as well as the geometry of drawing and computation conditions are summarized in table 1.
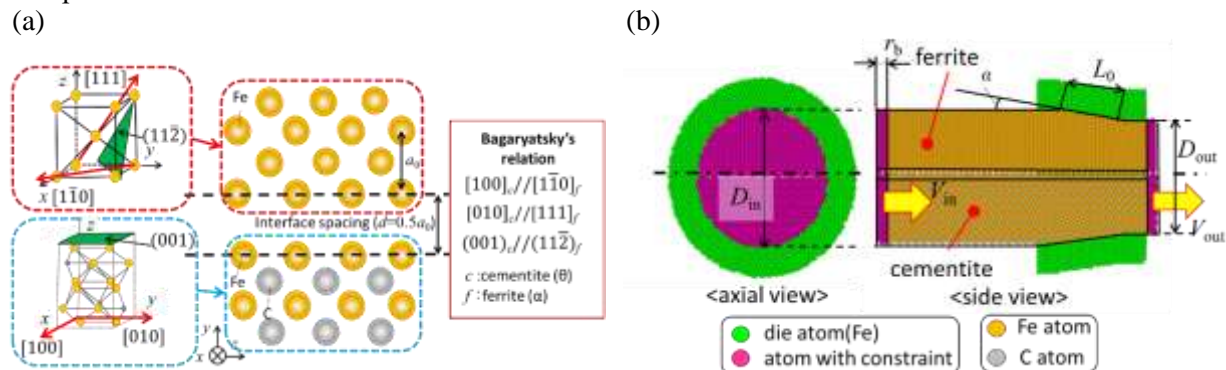
(a)   (b)

Figure 1. Nano-sized drawing model of pearlitic steel wire used for MD simulation. (a)Arrangement of crystal orientation of ferrite(α phase: α-Fe) and cementite (θ phase: Fe_3C) crystals at the interface (using Bagaryatsky's relation, here). (b)Configuration of two layers and geometry of drawing

Table 1. Geometry of drawing and MD computation conditions

Lattice constant (ferrite (α)) a_0 (nm)			0.28665
Lattice constant (cementite (θ)) a, b, c (nm)			0.4523, 0.5089, 0.6743
The number of atoms	total		77657
	Fe	cementite (θ)	22607
		ferrite (α)	22709
	C	cementite (θ)	7514
	die		24827
Die semi-angle α (deg)			7.0
Inlet diameter D_{in} (nm)			6.8796
Length of die land L_0 (nm)			4.12
Drawing velocity V_{in} , V_{out} (m s^{-1})			36.4, 50.0
Temperature T (K)			10, 600, 1000
Time increment $\times$ Steps			2.0 $\times$ 40000

3. Results and Discussion

3.1. Behaviour of carbon atoms near ferrite-cementite interface

Figure 2 shows occurrence of lattice defects during drawing by using CNA technique [14], which can make distinction between atoms with usual crystal (ordered) structure and with other (disordered) structure. Atoms in θ-phase are all identified as crystal defect because the CNA does not detect orthorhombic crystal that Fe_3C is supposed to have. The interface position shifts a little bit to easily deformable ferrite side, but it almost retains its original flat shape during drawing. As drawing begins, first the region with phase transition from bcc structure to face-centred cubic(fcc) structure takes place and expands particularly to front portion of the wire, and after then dislocation or grain boundary is left behind around the transition region.

Figure 3 shows time transition of normal stress in drawing direction (i.e. drawing stress) averaged over atoms in the wire. Stress increases rapidly at very beginning of drawing. By the completion of phase transition or formation of defects the drawing stress decreases rapidly, and after that it is kept at almost constant value. That stationary stress is regarded as a flow stress meaning plastic deformation. The smaller the system temperature is, the larger the flow stress is. From this fact we can guess that, in α-θ interface, C atoms are diffusing around θ phase side much more in higher temperature and enter into α phase side that much. When C atoms behave in such manner, they works as resistance of plastic deformation in ferrite phase, then hardening results in. This mechanism is rather similar to strengthening usually explained for the formation of martensite in Fe-C system.
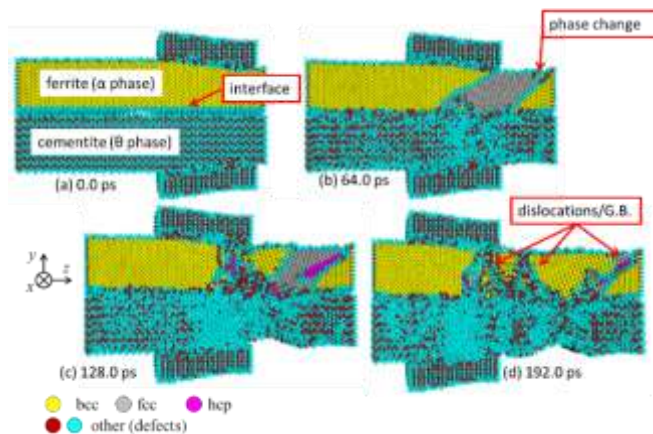
Figure 2. Deformation and lattice defects observed by CNA technique [14] in MD wiredrawing model of pearlite steel (viewing on cross-sections)
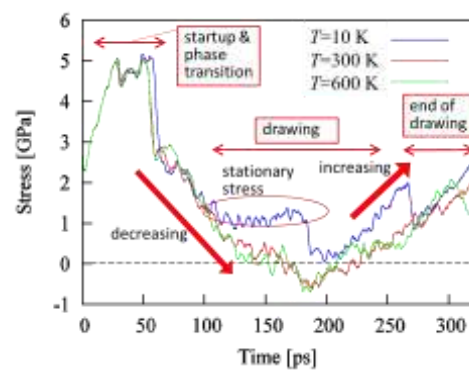
Figure 3. Time transition of averaged stress in drawing direction (drawing stress) during drawing process

3.2. Relation between dislocation motion and carbon diffusion (inspection of "drag mechanism")

Since we understand that C atom diffusion around the interface is key behavior for deformation process in pearlitic wire model, we observe position and trajectory of C atoms during drawing. Figure 4 shows time-evolution of the position of C atoms found in ferrite region at very close to the interface at *T*=10 K. The reason why observing in such low temperature is that, in high temperature like 1000 K, due to high diffusivity, C atoms move rapidly and are not captured at a stationary position.
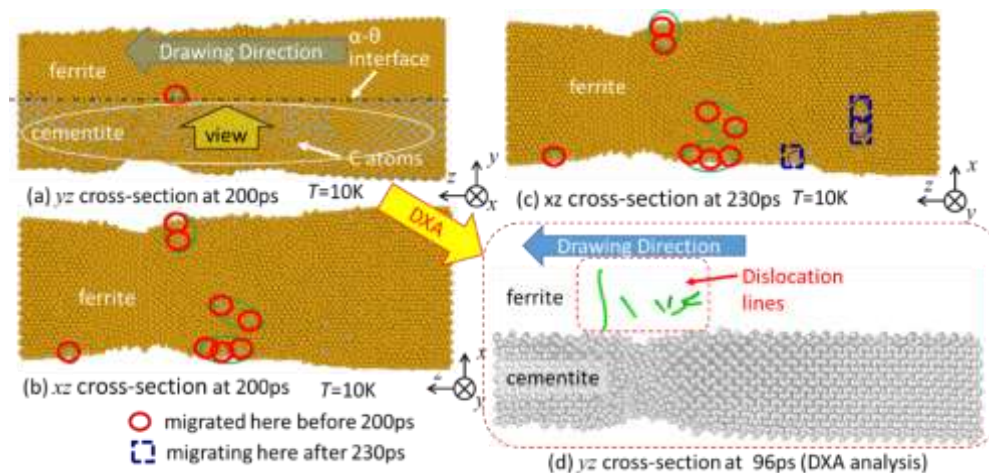

Figure 4. (a),(b),(c)Change of positions of carbon atoms around θ-α interface at which drawing stress rises again, and (d)position of carbon atoms and dislocations lines detected by DXA method [12]

Let us compare results between at times 200 ps (figure 4(a),(b)) and 230ps (figure 4(c)) (time means duration after the start of processing), at which drawing stress rises again from the saturated flow stress. The number of C atoms detected there are increasing. This movement of C atoms is probably being caused by plastic deformation in drawing. In literature, there was a proposal of mechanism that dislocation movement supports the travel of C atoms from θ phase to α phase, which can be called "drag mechanism (by dislocation motion)" [15]. However from the present MD simulation, as shown in figure 4(d), dislocation lines do not observed not so much even in low temperature case (figure 4(d) is obtained as the maximum appearance of dislocations). We can conclude that C atoms are certainly diffusing very much around the interface and such diffusive C

atoms can help the wire in resisting to drawing deformation (more generally, plastic deformation), but it is not directly linked to dislocation motion as in "drag mechanism." However, at this point any plastic deformation in θ phase has not captured. We think it needs further discussion and is left to further study.

4. Conclusion

In this study, by using molecular dynamics simulation, possibility of nano-sized wiredrawing of metals was investigated. Although the friction between die and wire atoms tends to become tremendously larger, in MD models using artificial lubrication mechanism drawing is theoretically possible. Pearlitic steel model with two layer of cementite and ferrite were successfully simulated. At the interface carbons diffuse around the interface and work as resistance to drawing stress and plastic deformation. However, "drag mechanism" by dislocation proposed for cementite decomposition mechanism, was not confirmed by the present atomistic scale.

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