

Molecular Dynamics Simulation of Melting of Thin γ Fe-C Films Having (100), (110) and (111) Surfaces

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Melting is a phase transition relevant to materials processing. The first interest in melting is about the site where melting starts, which site is known to be a surface since there is nucleation of liquid occurring on the surface at temperatures lower than the melting point [1]. This phenomenon is known as surface melting, which was firstly observed for Pb using the medium-energy ion scattering technique [2]. The surface-melting layer is essentially a solid phase because it has the structural periodicity of crystals; nevertheless, atoms in the surface-melting layer have large mean square displacements comparable to those of atoms in liquid, and thus this layer also seems close to liquid from the perspective of atomic movements [3]. Furthermore, it has been shown that surface melting displays surface orientation dependence both experimentally and theoretically; for example, it has been demonstrated that for fcc metals with (110) surface shows surface melting but those with (111) surface do not. For a system having larger specific surface area, *e.g.*, thin films, nano-particles *etc.*, it is likely that surface melting lowers its melting temperature more prominently. Kojima and Susa [4] have simulated melting of thin Cu film models having (100), (110) and (111) surfaces by molecular dynamics (MD) simulation and found that the melting temperature of the (110) model is lower than the others' because surface melting occurs in the (110) surface. However, there have been no reports about surface melting of alloys so far. Thus, the aim of the present work is to investigate melting dynamics of γ Fe-C alloy by MD to explore a possibility of surface melting being applied to nano-materials processing.

Structures of thin film models of γ Fe (88 Å thick) having (100), (110) and (111) surfaces containing about 0 - 4 at% C were calculated by constant temperature MD in the temperature range 1000 - 1800 K.

The liquidus temperature for each thin film model, determined as the temperature where the discontinuous change in internal energy was observed, decreased with increasing the C concentration, which corresponds to the decrease of the liquidus temperature for γ Fe with an increase in the C concentration on the Fe-C phase diagram.

Figure 1 shows number density distributions of Fe and C atoms for the (110) thin film model of γ Fe containing 4 at% C at 1400 and 1560 K. Values of $\rho(z)$ for C are expressed as those multiplied by five. The origin on the abscissa is located at the center of the unit cell, and the arrow represents the surface layer at 1000 K. The peaks for Fe near the surface are lower than those inside at 1400 K and further decrease with increasing temperature. These findings say that atomic movements are stronger near the surface than inside and are enhanced by a temperature rise. Furthermore, at 1560 K there are no distinct peaks near the surface, which indicates that there is a liquid phase formed, solid and liquid phases containing C coexisting at this stage. Inspection of Figure 1 shows that the temperature rise increases the number density of C atoms near the surface and, as a result, the presence of C

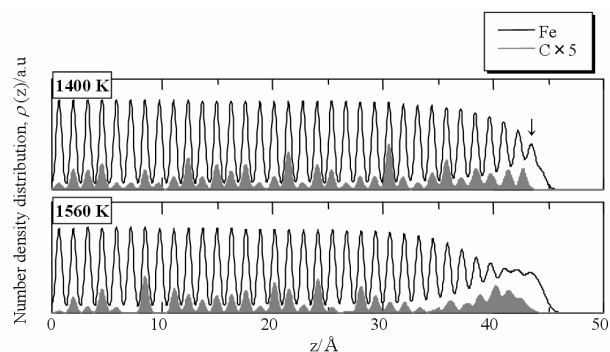


Figure 1 Number density distributions of Fe and C atoms of γ Fe (110) thin film model containing 4 at% C.

between Fe atoms weakens the attractive force between Fe atoms, which would cause the thin film models of γ Fe-C alloy to melt at temperatures lower than γ Fe. Accordingly, it is also likely that surface melting of γ Fe-C occurs at temperatures lower than pure γ Fe. To confirm this, the thickness of the surface-melting layer is estimated on the basis of Lindemann's law, which is expressed by the following equation [5,6]:

$$\langle u^2 \rangle = (\delta d)^2$$

where $\langle u^2 \rangle$ is the mean square amplitude of atomic vibrations, d is the nearest atomic distance at the melting point and δ is a constant specified by the element. The value of δ for γ Fe has been obtained as 0.08457 at the melting temperature using (111) thin film model [7]. Assuming that melting of γ Fe-C alloy is equivalent to melting of γ Fe, the surface melting layer thickness for γ Fe-C is obtained as the thickness of the surface layer having $\langle u^2 \rangle$ greater than that derived from Lindemann's law. It has been concluded that surface melting occurs in γ Fe-C alloy, in particular, in γ Fe having (110) surface more easily.

To confirm whether surface melting works effectively for melting of Fe at lower temperatures, MD simulation was carried out for the carburization process in the (111) and (110) thin film models of pure γ Fe in equilibrium at 1600 K for 500 ps. The diffusion distance of C during this period was longer in the (110) thin film model. This is because the (110) thin film model has a thicker surface-melting layer in the initial condition and the diffusion coefficient of C in the surface-melting layer is greater than that in the solid phase, since the surface-melting layer is close to liquid in terms of atomic movements.

Consequently, surface melting would work more effectively in melting and joining processes for nano-particles as well as nano thin films, in addition to nano-structured objects, under optimized conditions of the dimensions and surface orientations of materials.

References

- [1] J.N. Stranski, *Naturwissenschaften* **29** (1941) 743
- [2] J.W. Frenken M, J.F. van der Veen, *Phys. Rev. Lett.* **54** (1985) 134-137
- [3] J.F. van der Veen, B. Pluis, A.W. van der Gon, in R. Vanselow, R.F. Howe (Eds.), *Chemistry and Physics of Solid Surfaces VII*, Springer Series in Surface Sciences, Vol. 10, Springer, Heidelberg, (1988) 455-490
- [4] R. Kojima, M. Susa, *High Temperatures-High Pressures* **34** (2002) 639-648
- [5] F.A. Lindemann, *Z. Phys.* **10** (1910) 609-612
- [6] J.J. Gilvarry, *Phys. Rev.* **102** (1956) 308-316
- [7] R. Kojima, M. Susa, *Sci. Tech. Adv. Mat.* (in press)