Influences of Lattice and Bond Strain on Nucleation-Triggered Massive-like δ-γ Transformation of Carbon Steel

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Phase transformation of carbon steel from δ phase to γ phase follows peritectic reaction when carbon concentration is between 0.1 and 0.51 mass% according to the Fe-C binary phase diagram. *In situ* observation of the transformation using synchrotron radiation, however, revealed yet another transformation, referred to as massive-like transformation, where δ phase directly transforms to γ phase without involving liquid phase [1]. Due to the difference in density between BCC-structured δ phase and FCC-structured γ phase and the absence of liquid phase which can accommodate strain due to the difference, it may accompany cracks on the surface of casted steel. Although the mechanism of this transformation has not been understood well enough to enable us to control the transformation to minimize any unwanted consequence, systematic atomistic analyses of the heterogeneous δ/γ interface between the two phases [2] and their impact on nucleation of γ phase in δ phase matrix [3] suggested that relatively high δ/γ interface energy for the entropy change upon the transformation is primarily responsible for the large undercooling required for the transformation. However, in those studies, another important factor, the difference in density or consequent strain, has not been taken into account, despite the fact that *in situ* observations showed non-uniform morphological change upon the transformation. Thus, in this study, atomistic simulations as well as numerical analyses for thermodynamics of nucleation have been carried out with the strain fully taken into account, to clarify the impact of the strain on nucleation of γ phase.

Driving force and energy barrier for nucleation are determined by δ/γ interface energy as well as strain energy associated with the volume change. Since FCC and BCC structures significantly differ from each other in terms of interatomic matching even when the mismatch is minimal as in well-known KS or NW orientation relationship, long-range matching between supercells comprised of repeated unitcells are examined to evaluate δ/γ interface energy as a function of the length of the supercell. Assuming that nucleating γ phase is isotropically strained without straining δ phase matrix, the volume elastic strain can easily be converted from the length of the supercell.

Figure 1 shows optimized atomic configuration in the supercell where a FCC slab adjoins a BCC slab satisfying the NW orientation relationship with minimal long-range mismatch. Although strain of individual bonds are not uniform along the interface, the bond strain is confined to approximately 5 Å at either side of the interface. Figure 2 shows interface energy, as a function of the supercell length, obtained by static lattice calculations using EAM interatomic potential with strained unitcells as standard states for both phases: contribution of lattice strain is intentionally excluded from the interface energy. Here, difference in the numbers of BCC and FCC unitcells along *y*- and *z*-axes in supercells is fixed to 1 as in Fig. 1. The strain-excluded interface energy is increased with the decrease of the supercell length due to increased bond strain imposed by the long-

range lattice mismatch. On the other hand, it is asymptotically decreased with the increase of the supercell length since atom-to-atom correspondence across the interface is improved when ratio of the numbers of unitcell approaches to unity, due to identical atomic configuration on (011) plane of BCC and (111) plane of FCC. Fig. 2 also shows elastic strain energy of 10 Å wide interface region for unit area (thus in the same unit as for interface energy) calculated using bulk modulus and aforementioned volume elastic strain, only for comparison, though its curvature changes with volume of the region assumed. These results qualitatively suggest that interface, and in turn, γ-nucleus, is stable only when lattice strain is nearly minimal. Finally, using the strain-excluded interface energy and volume elastic strain for a specific supercell exhibiting minimal mismatch (Fig. 1) or the volume elastic strain, free energy change upon nucleation and critical radius for it were calculated (Figs. 3 and 4). It is found that driving force for nucleation is not proportional to undercooling, but it has threshold before which nucleation is thermodynamically inhibited, even when the volume elastic strain is nearly minimal. These results explain the experimental fact that large undercooling is required for massive-like transformation from δ phase to γ phase.

References

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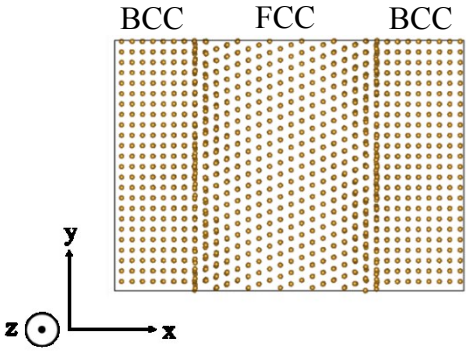

Fig. 1 An example supercell of δ/γ interface and optmized atomic configuration. Distortion of bond was confined within 5 Å at either side of the interface.

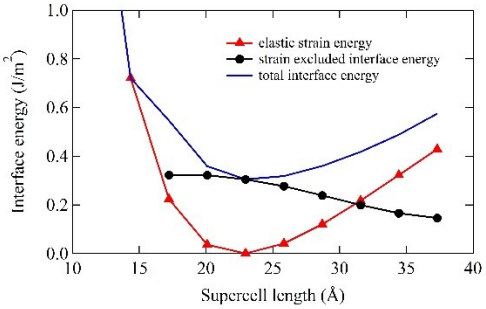

Fig. 2 Strain-excluded interface energy as a function of supercell length along *z*-axis, in comparison with cell strain energy in 10 Å wide interface region.

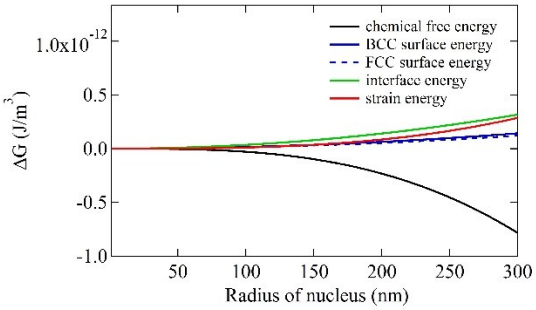

Fig. 3 Free energy change upon nucleation as a function of radius of nucleus at ΔT = 100 K.

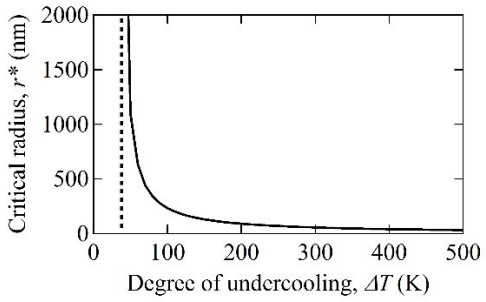

Fig. 4. Critical radius as a function of undercooling. Dashed line at ΔT ~ 30 K indicate threshold for nucleation.