

Stability and strength of bcc-Fe / MX ($M=Nb, V, X=C, N$) interface in high-Chromium heat resistant martensitic steel

Kaoru Nakamura¹, Susumu Yamada¹, Toshiharu Ohnuma¹

¹ Central Research Institute of Electric Power Industry, 2-6-1, Nagasaka, Yokosuka, Kanagawa 240-0196, Japan

9–12 % Cr martensitic stainless steel (high-Cr steel) has been applied for recent USC (ultra super critical) fossil power plant as steam pipes, because of its superior high-temperature strength. Fine precipitates, such as $M_{23}C_6$ ($M=Fe, Cr$) and MX ($M=Nb, V, X=C, N$), are responsible for the creep strength of high-Cr steel by the pinning of the dislocation motion. However, creep strength of high-Cr steel is prospected to be significantly decreased under long time operation ($\sim 10^5$ hr operation at 873 K). Coarsening of $M_{23}C_6$, re-resolution of MX and Z-phase (CrNbN or CrVN) precipitation is reported to play significant role to decrease the creep strength [1]. Especially, Z-phase precipitates only under long-time creep condition, and is suggested to precipitate from MX [2].

However, long-term stability of MX and detailed precipitation mechanism of Z-phase is still unclear, because of the limited investigation of atomic scale for high-Cr steel. Long-time creep life prediction of high-Cr steel requires proper modelling of precipitation changes and its effect on the creep damage. Thus, in this study, first-principles calculation was utilized to investigate Fe / MX ($M=Nb, V, X=C, N$) interface in order to understand the phase stability of MX and precipitation mechanism of Z-phase.

Figure 1 (a) shows the Fe / VC interface with Baker-Nutting orientation relationship. Consideration of the rigid body translation within the interface revealed that Fe-C ontop configuration is most stable, the same as Fe / V_4C_3 interface [3]. Theoretical stress-strain curves of both Fe / VC and Fe / V_4C_3 interfaces are shown in Fig. 1 (b). Ideal interfacial strength (Maximum stress) of Fe / VC interface is higher than that of Fe / V_4C_3 interface, while the latter shows more ductility because of the electron redistribution from the ordered C vacancies. Fig. 2 (a) and (b) shows the migration path of C from VC to Fe across the interface, and corresponding energy profile calculated by NEB (Nudged Elastic Band) method, respectively. Although the C needs to overcome high migration barrier (~ 1.8 eV) across the interface, it is lower than the migration energy of C in VC (~ 2.4 eV). These results indicate that interfaces between parent phase (bcc-Fe) and MX precipitates are responsible for degradation of high-Cr steel.

Moreover, Cr was found to segregate at Fe / MX interface by systematically calculated substitutional formation energy of Cr for metal sites. This finding supports that Z-phase precipitates at Fe / MX interface, because the crystal structure of Z-phase is represented as the stacking of bcc-Cr layers and VN (or NbN) layers. Detailed atomistic precipitation mechanism and effect of the Z-phase precipitation on the mechanical property will be discussed at the conference.

References

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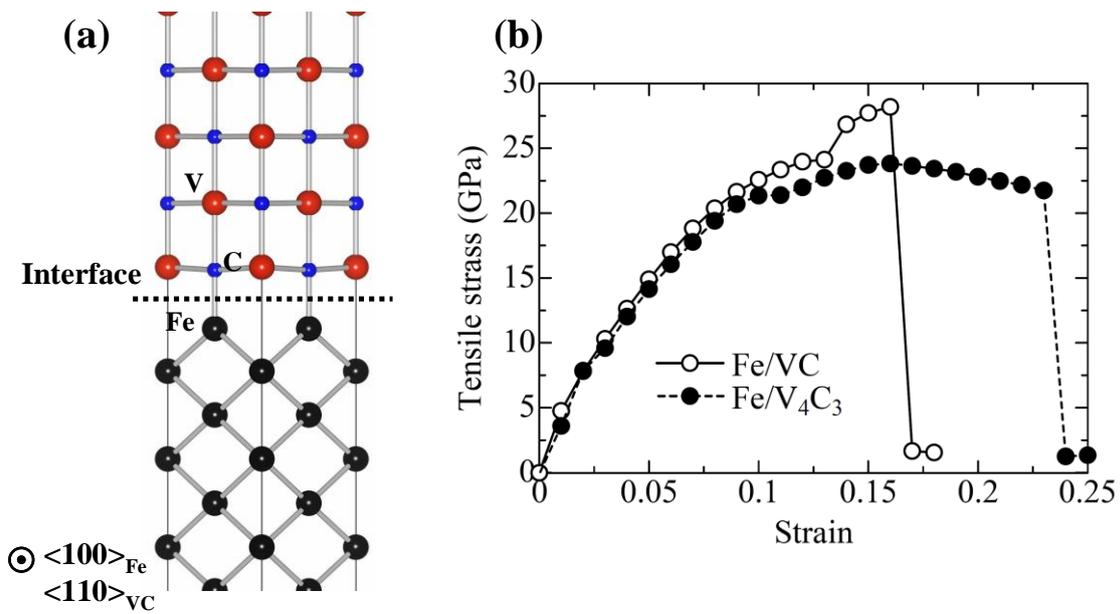


FIG. 1. (a) Schematic illustration of bcc-Fe / VC interface, (b) theoretical stress-strain curves for Fe / VC and Fe / V₄C₃ interfaces.

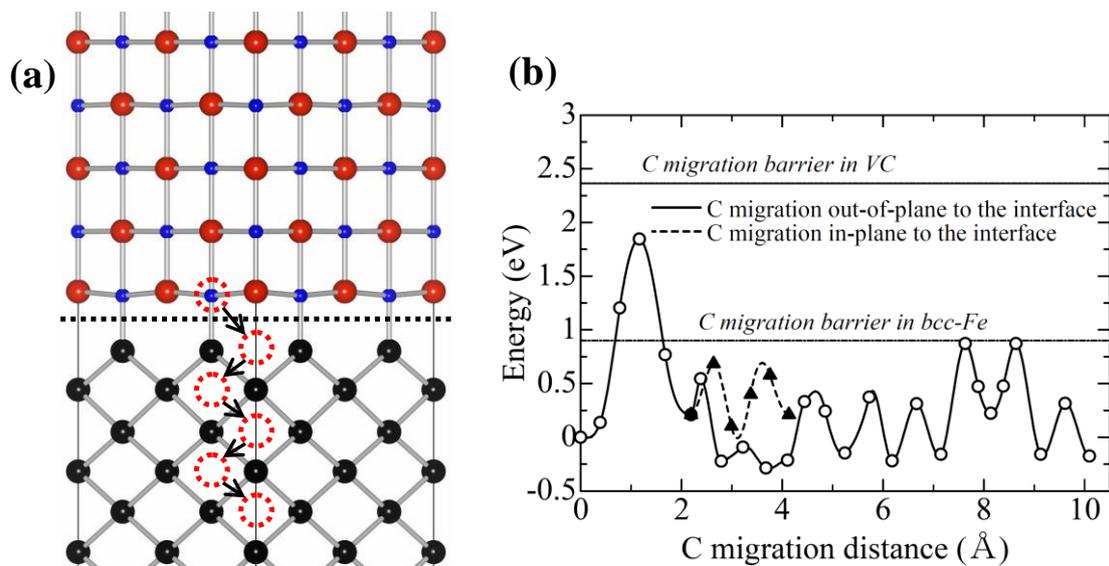


FIG. 2. Migration path of C from VC to bcc-Fe across the interface, (b) energy profile of C migration.