The microstructural evolution of c-type dislocation loop in zirconium and the effects of iron atoms on the formation process

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Abstract

The formation process of c-type dislocation loop, which is observed to form at almost the same time with the abrupt increase in hydrogen absorption of Zr alloys used in nuclear reactor, has been evaluated by molecular dynamic simulation. The different conversion path of the vacancy cluster aggregation and the effect of iron atoms have been discussed.

Keywords: zirconium, molecular dynamics simulation , irradiation induced defects

1. Introduction

The formation of c-type dislocation loop with Burgers vector $1/6[20\bar{2}3]$[1] is believed to have a close relationship with the hydrogen pickup happened in the Zr alloys used in fuel claddings under operating temperature. Meanwhile, the alloying elements play an important role on the formation of the c-loops, especially the iron atoms. The partially dissolved second phase particles (SPPs) and the segregation of Fe atoms to the c-loops have been observed experimentally.[2] But the influence of iron atoms on the formation of c-loops remains unclear. In this research, the microstructural evolution of c-type dislocation loop has been observed and effect of iron atoms has been discussed.

2. Calculation Method

The Mendelev potential#3 and the Zr-Fe potential based on the Mendelev potential#3 have been used by Lammps code[3] in molecular dynamic simulation. The size of the Zr lattice is X$[1\bar{1}00]$ 19.6nm, Y$[11\bar{2}0]$22.6nm and Z[0001] 18.1nm. In the center of the lattice, the hexagonal vacancy cluster with 10~13 atoms every edge has been inserted and the system has been minimized under 600K. The system has been minimized every 10 timesteps to obtain the conversion path of the vacancy cluster aggregation. Also, when the Fe atoms uniformly distributed at the edge of the c-type dislocation loop as the interstitial site, the energy difference caused by the formation of c-loops has been calculated compared with the pure Zr cell. The number of Fe atoms is half of the number of vacancies at the edge.

3. Results and Conclusions

During the process of vacancy cluster aggregation, there are two conversion paths. One conversion path is that the atoms collapse directly along the z axis without movement along the basal plane. Another conversion path is that the atoms move along the basal plane during the collapse process to form the partial displacement within x-y plane.

The figure 1 shows that the raise of energy caused by the formation of c-loops is higher when the Fe atoms segregate to the edge of the c-loops. The iron atoms seem to impede the formation of c-loops.

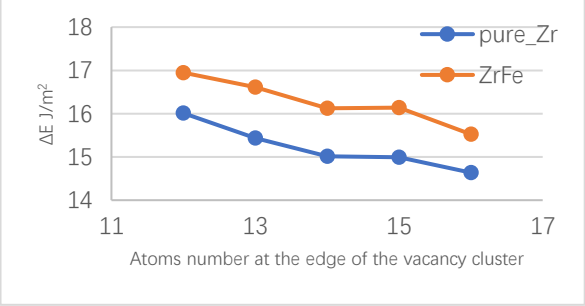

Figure 1 The energy difference between perfect hcp structure and lattice with c-loops

References

[1] R.A. Holt, R.W. Gilbert, J. Nucl. Mater. 137 (1986) 185-189.

[2] Y. de Carlan, C. Regnard, M. Griffiths, in: Zircon. Nucl.Ind. Elev. Int. Symp., 1996: pp. 638–653.

[3] <http://lammps.sandia.gov>

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