Conf-901105 57

CONF-901105--57

DE91 006033

CALCULATION OF DEFECT PROPERTIES OF NiTi AND FeTi*

Russell T. Lutton and Michael J. Sabochick
Air Force Institute of Technology
Dept. of Engineering Physics
Wright Patterson AFB, OH 45433
and
Nghi Q. Lam
Materials Science Division
Argonne National Laboratory
Argonne, IL 60439

December 1990

The submitted manuscript has been authored by a contractor of the U.S. Government under contract No. W-31-109-ENG-38. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Presented at the Materials Research Society Fall Meeting, Symposium K: *Defects in Materials*, Nov. 26-30, 1990, Boston, MA.

*Work supported by the U. S. Department of Energy, BES-Materials Sciences, under Contract W-31-109-Eng-38 and from the Air Force Institute of Technology.

MASTER

[illegible] OSTI

JAN 1

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

CALCULATION OF DEFECT PROPERTIES OF NiTi AND FeTi

RUSSELL T. LUTTON[1], MICHAEL J. SABOCHICK[1†] and NGHI Q. LAM[2]

[1]Air Force Institute of Technology, Department of Engineering Physics,
Wright-Patterson Air Force Base, OH 45433-6583
[2]Argonne National Laboratory, Materials Science Division, Argonne, IL 60439

ABSTRACT

The energies and configurations of interstitials and vacancies in the B2 ordered compounds NiTi and FeTi were calculated using atomistic simulation. The stable configuration of a vacancy after the removal of an Ni atom was a vacant Ni site; similarly, the removal of an Fe atom in FeTi resulted in a vacant Fe site. Removal of a Ti atom in both compounds, however, resulted in a vacant Ni or Fe site and an adjacent antisite defect. The effective vacancy formation energies in NiTi and FeTi were calculated to be 1.48 and 1.07 eV, respectively. Interstitials in NiTi formed split <111> configurations consisting of a Ni-Ni dumbbell oriented in the <111> direction with one or two adjacent antisite defects. The Fe interstitial in FeTi had a similar configuration, except the dumbbell contained Fe atoms. The Ti interstitial in FeTi formed an <110> Fe-Fe dumbbell.

INTRODUCTION

A recent computer simulation study of the crystalline-to-amorphous (C-A) transition of Cu_mTi_n compounds under electron irradiation indicated that point defects were a critical factor in the transition [1,2]. In an accompanying study of point defects in CuTi and $CuTi_2$, it was found that the stable interstitial configurations consist of Cu atoms in a split <111> interstitial, surrounded by one or more antisite defects [3]. From the observation that these configurations were rather complicated, it was presumed that interstitials in the compounds were less mobile than their pure metal counterparts. This could explain how point defect concentrations can increase sufficiently during electron irradiation to induce amorphization [3].

The purpose of the present work was to calculate the point-defect properties of NiTi and FeTi. These properties are compared with those calculated for the Cu_mTi_n compounds, and the implications regarding amorphization are discussed. In computer simulation studies of the amorphization of NiTi and FeTi, it has found that point-defect introduction is necessary to trigger the C-A transition [4,5]. The findings for FeTi were similar to those for the Cu_mTi_n compounds; the chemically-disordered state had a lower energy than the amorphous state [4]. In NiTi, however, chemical disorder alone was capable of storing enough energy to favor the transition, although, as in the other compounds, the transition was not observed without point defect introduction [5].

METHOD

The computational methods employed in the present work were molecular statics, molecular dynamics and Monte Carlo, using a modified version of the code DYNAMO [6]. The simulations used a fixed cubic volume containing $N = 1024$ atoms and having periodic boundaries.

[†] To whom correspondence should be addressed.

Lutton et al. '94

The interatomic potential functions were determined using a modification of the method of Oh and Johnson [7]. The potentials for pure Fe, Ni and Ti were fitted to the binding energy, lattice constants, elastic constants and vacancy formation energy of the pure elements. The potentials for Fe-Ti and Ni-Ti were then fitted to the structure, lattice constants and heat of formation of the compound. The fitting procedure was identical to that described in [2]; the details for NiTi and FeTi are discussed elsewhere [5].

All of the defect properties were calculated using molecular statics, i.e., by minimizing the energy of various trial configurations. As is the case in pure metals, the minimum-energy configurations of interstitials were more difficult to determine than those of vacancies. In compounds, this is also complicated by the fact that these configurations may contain one or more antisite defects [3]. To allow these antisite defects to form, the systems were heated to 500-700K in Monte Carlo runs, and atoms of different types were allowed to switch positions.

VACANCY PROPERTIES

The energy of the 1024-atom perfect lattices were calculated to be $U_0 = -5120.861$ and -5008.453 eV in NiTi and FeTi, respectively. The simplest defect in a substitutional alloy is an antisite defect, where an atom is on a lattice site but is of the wrong type. The calculated energies of these systems are given in Table 1. The formation energy of an antisite pair was calculated to be 1.015 and 0.726 eV in NiTi and FeTi, respectively.

For the purpose of discussion, let us consider a B2 compound consisting of X and Y atoms. The B2 structure is a bcc lattice with an X atom in the center of the unit cell and Y atoms at the corners. An X vacancy is created by removing an X atom; let us define a type-A configuration for an X vacancy as simply a vacant X site. A type-B configuration is created when an adjacent Y atom moves into the vacant X site, and thus consists of a vacant Y site and an antisite defect at a first-nearest-neighbor X site. For a Y vacancy, of course, one interchanges X and Y in these definitions.

In NiTi, the lowest energy configuration of the Ni vacancy was found to be type-A; the energy of this and other stable configurations are listed in Table 1. The lowest-energy configuration of the Ti vacancy, however, was found to be type-B. The difference in energy between the type-A and type-B configurations was found to be 0.205 eV; the migration barrier from type-A to type-B was calculated to be 0.134 eV. The antisite defect and vacant Ni site in the type-B configuration were found to be weakly bound with a binding energy of 0.094 eV.

The vacancy configurations in FeTi were found to be essentially identical to those in NiTi. The stable Fe vacancy was found to have a type-A configuration. The stable Ti vacancy configuration was type-B, with an energy difference of 1.028 eV between the type-A and type-B configuration. The migration energy barrier from the type-A to the type-B configuration was calculated to be 0.341 eV. As with the Ti vacancy in NiTi, the vacant Fe site and the antisite defect in the type-B configuration were found to be weakly bound with a binding energy of 0.055 eV.

The formation energies of defects are more difficult calculate in compounds than they are in pure systems, because the removal or addition of an atom changes the stoichiometry. Foiles and Daw [8], however, proposed a method which was used here to calculate the vacancy concentrations over a wide range of temperatures. If the concentrations have an Arrhenius behavior, effective formation energies may be calculated [3]. Such was the case, and the effective vacancy formation energy was calculated to be 1.48 and 1.07 eV in NiTi and FeTi, respectively.

Table 1. Stable Defect Configuration Energies.
Energies are with respect to a 1024-atom perfect lattice.

System	Number of Atoms	$E = U - U_0$ [eV] NiTi	FeTi
Ni or Fe on Ti site	1024	0.762	0.491
Ti on Ni or Fe site	1024	0.253	0.235
Ni or Fe Vacancy	1023	6.356	5.900
Ti Vacancy	1023	7.024	6.336
Ni or Fe Interstitial	1025	-2.395	-1.558
Ti Interstitial	1025	-2.602	-1.945

The migration of an Ni and Fe vacancy consists of a six-jump ring mechanism, translating the vacant Ni or Fe site to another Ni or Fe site at a second-nearest neighbor location. The migration energies through this mechanism were calculated to be 1.272 and 1.738 eV in NiTi and FeTi, respectively. These values are relatively large compared to typical vacancy migration energies in pure metals because the intermediate configurations contain antisite defects and/or a vacant Ti site.

INTERSTITIAL PROPERTIES

Interstitials in NiTi and FeTi were found to occur in one of two possible configurations. The first was found to be the lowest energy configuration of the Ni and Ti interstitials in NiTi (differing only in the number of neighboring antisite defects), and the Fe interstitial in FeTi. This configuration consisted of an Ni-Ni or Fe-Fe dumbbell, oriented in the <111> direction and centered on a Ti site, which had one or two adjacent antisite defects (Ti atoms on Ni or Fe sites). We term this configuration a <111> split interstitial, as there was found to be considerable displacement of atoms along the <111> direction.

The Ti interstitial in FeTi was found to be most stable in the second interstitial configuration, which was similar to the first except that the Fe-Fe dumbbell was oriented along a <110> direction. The displacement of nearby atoms was also considerably less in this configuration. Two antisite defects (Ti atoms on Fe sites) were adjacent to the dumbbell.

DISCUSSION

A summary of the calculated defect properties of NiTi, FeTi, CuTi and $CuTi_2$ is given in Table 2. NiTi has the largest antisite-pair energy--more than 0.6 eV higher than the correponding values in CuTi and $CuTi_2$. This explains the why chemical disordering can store a large amount of energy in NiTi as was found in the study of the C-A transition of this compound [5].

The vacancy configurations found here for NiTi and FeTi are similar to those found in CuTi and $CuTi_2$. In the latter compounds, a Cu vacancy was type-A, and a Ti vacancy was type-B [3]. However, the calculated vacancy migration energies were considerably larger than the corresponding energies in CuTi and $CuTi_2$. This is partially explained by the fact that antisite defects are formed during the various jump mechanisms, and the antisite defect energy is larger in NiTi and FeTi than it is in CuTi and $CuTi_2$.

Lutton et al. 3/4

Table 2. Calculated Point Defect Energies.

	Energy [eV]			
	NiTi	FeTi	CuTi[a]	CuTi$_2$[a]
Antisite pair	1.015	0.726	0.385	0.460
Ni, Fe, or Cu Frenkel pair	3.961	4.341	2.769	2.776
Vacancy Migration	1.272	1.738	0.19/1.32	0.92
Vacancy Formation	1.480	1.070	1.09	0.90

[a] Ref. 3.

Except for the Ti interstitial in FeTi, the interstitial configurations of NiTi and FeTi are similar to those found for CuTi and CuTi$_2$. In the latter compounds, the interstitial consisted of a Cu-Cu dumbbell roughly centered on a Ti site, oriented in the <111> direction, and surrounded by one or more antisite defects [3]. The Ti interstitial in FeTi is apparently unique since it was found to contain a <110> dumbbell. All interstitial configurations, however, contained antisite defects, which probably results in relatively large migration energies.

CONCLUSIONS

The point defect properties of NiTi and FeTi were calculated using atomistic simulation. Many parallels were found between the point defects in these compounds and those in CuTi and CuTi$_2$, such as similar vacancy and interstitial configurations. The fact that the interstitial configurations were found to be relatively complicated suggests that these point defects are less mobile in compounds than in pure elements. The antisite-pair energy was found to much higher in NiTi than in CuTi and CuTi$_2$, explaining the large chemical-disordering energy recently found in simulations of the C-A transition in NiTi.

ACKNOWLEDGEMENTS

Part of this work was performed at Argonne National Laboratory while one of us (MJS) was a Faculty Research Participant supported by the Argonne Division of Educational Programs. Support from the Air Force Institute of Technology and the U.S. Department of Energy, BES-Materials Sciences, under Contract W-31-109-Eng-38, gratefully acknowledged.

REFERENCES

1. M. J. Sabochick and N. Q. Lam, Scripta Met. et Mater. **24**, 565 (1990).
2. M. J. Sabochick and N. Q. Lam, Phys. Rev. B, accepted for publication.
3. J. R. Shoemaker, R. T. Lutton, D. Wesley, W. R. Wharton, M. L. Oehrli, M. S. Herte, M. J. Sabochick and N. Q. Lam, J. Mater. Res., accepted for publication.
4. M. J. Sabochick and N. Q. Lam, to be published.
5. M. J. Sabochick and N. Q. Lam, presented at the Mater. Res. Soc. Fall Meeting, Symposium A: Surface Chemistry and Beam-Solid Interactions, Boston MA, Nov. 26-30, 1990.
6. M. S. Daw, M. I. Baskes and S. M. Foiles (private communication).
7. D. J. Oh and R. A. Johnson, J. Mater. Res. **3**, 471 (1988).
8. S. M. Foiles and M. S. Daw, J. Mater. Res. **2**, 3 (1987).

END

DATE FILMED

01 / 23 / 91