ATOMISTIC POTENTIAL FOR MARTENSITIC TRANSFORMATIONS IN CUALNI

Yubao Zhen, Chengbiao Chu
Department of Astronautical Science and Mechanics, School of Astronautics, Harbin Institute of Technology, Harbin, 150001, P.R. China

Summary The second nearest-neighbor modified embedded atom method (2NN MEAM) for ternary shape memory alloy CuAlNi is developed to simulate the martensitic transformations. Pairwise potential for the base binary alloy CuAl with DO3 reference structure (Cu3Al) is derived. Genetic algorithm and finite temperature effect are incorporated in a potential parameter optimization package. The potential determined reproduces the martensitic transformations and mechanical properties calculated match those from experiments.

INTRODUCTION

Copper-based ternary alloy CuAlNi is a typical low-cost shape memory alloy with wide application temperature range. The dynamics of the underlying martensitic transformation (MT) is of fundamental importance but is very difficult to study experimentally. In this case, the atomistic approach offers a way for detailed understanding and alloy design. However, two challenges hinder the application of such atomistic models for MT. One is from the multicomponent character, which demands enormous computation on elements and sub-alloy systems. The other is from the requirement to reproduce both forward and reverse martensitic transformations. Literature work on atomistic potential of CuAlNi is thus very limited.

METHODOLOGY

In this work, a second nearest-neighbor modified embedded atom method (2NN MEAM) is utilized for CuAlNi. To generate reliable potential parameters, with consideration of the thermoelastic nature of MT, we follow three strategies: parameter optimization with a genetic algorithm, determination of elastic constants only at finite temperatures [1], and adoption of DO3 (being also the structure of CuAlNi in austenite) as the reference structure of Cu-Al. A sophisticated MATLAB package incorporated with LAMMPS [2] and genetic algorithm [3] is developed for automated parameter optimization. Matching conditions are weighted and include elastic constants, structural energy difference and vacancy energy (for pure elements). In all cases, lattice stability and reproduction of MT phenomena are given the top priority.

DO3 reference structure

Reference structures and corresponding compositions for the three binary alloys Cu-Al, Cu-Ni and Al-Ni are taken as DO3 (Cu3Al), L12 (Ni3Cu), and B2 (AlNi), respectively. As a typical example, an alloy of Cu-14.2Al-4.3Ni (wt%) [4] (approximately Cu-27.96Al-3.89Ni (at%)) is considered. In CuAlNi, the most important sub-alloy Cu-Al (in Cu3Al) also shows MT behavior. In the framework of MEAM, the pair potential $\phi_{AB}(R)$ between AB for A3B (in DO3) is derived as

$$\phi_{AB}(R) = \psi(R) + \sum_{n=1}(-1)^n \left(\frac{Z_2}{Z_1}\frac{S_B + S_A^{EI}}{2}\right)^n \psi(a^n R), \tag{1}$$

$$\psi(R) = \frac{1}{2}E^u_{A3B}(R) - \frac{1}{8}F_A(\bar{\rho}_A^{0EI}(R)) - \frac{1}{4}F_A(\bar{\rho}_A^{0Q}(R)) - \frac{1}{8}F_B(\bar{\rho}_B^0(R)) - \phi_{AA}(R) - \frac{3}{4}S_A^Q\phi_{AA}(aR), \tag{2}$$

where $S_B = S_A^{EI}$ is the screening function for the 2NN A-B pair, $Z_1 = 8$, $Z_2 = 6$, and $a = 2/\sqrt{3}$ is the ratio of 2NN to 1NN distances. 'EIQ' are three location types: 'E' for $(1/2, 0, 0)$, 'I' for $(1/2, 1/2, 1/2)$, and 'Q' for $(1/4, 1/4, 1/4)$.

Special handling of copper

Copper, as a pure element, has a FCC lattice structure. However, in Cu3Al (and in CuAlNi as well), copper also presents a BCC sub-lattice, as shown in Fig. 1 (see the core of the DO3 supercell). This implies intrinsic instability and poses a driving force for MT. It also causes complexities in parameter determination. Setting $C_{\min} = 0$ and $C_{\max} = 2.8$ for copper proves to work for both FCC and BCC.

Table 1. The 2NN MEAM parameters for pure elements Cu, Al, Ni

	b_0	b_1	b_2	b_3	A	t_1	t_2	t_3	$C_{\min}$	$C_{\max}$	d_{attr}	d_{repuls}
Cu	3.61	2.38	5.67	2.30	0.88	2.68	2.94	2.26	0.0	2.8	0.05	0.05
Al	3.33	2.64	5.44	2.80	1.25	3.23	0.80	8.75	0.0	2.8	0.03	0.08
Ni	3.02	1.50	5.90	1.51	0.95	3.01	2.74	4.26	0.0	2.8	0.05	0.05

a) Corresponding author. E-mail: zhenyb@hit.edu.cn.

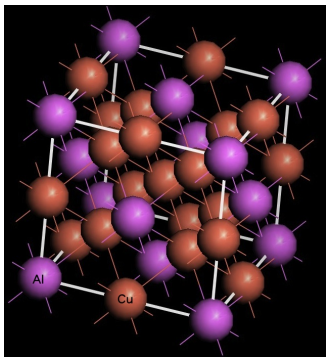

Figure 1. The DO3 structure of Cu3Al.

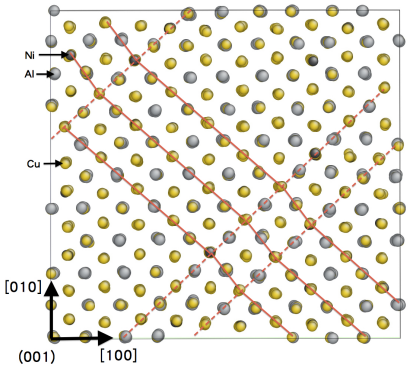

Figure 2. Twinned martensites after quenching.

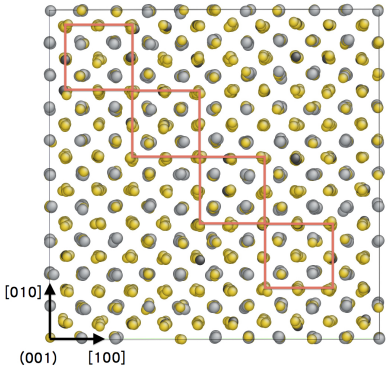

Figure 3. Austenite recovered when heated.

RESULTS

The 2NN MEAM potential parameters determined for pure elements, binary alloys, and ternary alloy are given in tables 1, 2, and 3, respectively. The electron density scalings are determined as $\rho^0_{\mathrm{Cu}} : \rho^0_{\mathrm{Al}} : \rho^0_{\mathrm{Ni}} = 1.0 : 1.65 : 1.0$. Elastic constants of all elements and alloys show good match to experimental values (data are not given here to save space).

Table 2. The 2NN MEAM parameters for binary alloys of Cu-Al-Ni

alloy i-j	E_c eV	r_e Å	B 10^{12} dyn/cm^2	α	d_{attr}	d_{repuls}	C^{iji}_{min} C^{iji}_{max}	C^{jij}_{min} C^{jij}_{max}	C^{iij}_{min} C^{iij}_{max}	C^{ijj}_{min} C^{ijj}_{max}
Cu-Al	3.84	2.5201	1.29	4.8281	0.03	0.07	0.64	0.51	0.12	0.16
							2.70	2.54	1.78	2.54
Al-Ni	4.52	2.4820	1.58	4.8025	0.02	0.07	0.22	0.72	0.93	0.35
							2.00	2.15	3.00	2.34
Cu-Ni	4.25	2.506	1.84	5.1997	0.05	0.05	0.78	0.85	1.52	0.68
							2.8	2.8	2.8	2.8

Table 3. The 2NN MEAM parameters for ternary alloy CuAlNi

$C^{\mathrm{Cu-Al-Ni}}_{\mathrm{min}}$	$C^{\mathrm{Al-Cu-Ni}}_{\mathrm{min}}$	$C^{\mathrm{Cu-Ni-Al}}_{\mathrm{min}}$	$C^{\mathrm{Cu-Al-Ni}}_{\mathrm{max}}$	$C^{\mathrm{Al-Cu-Ni}}_{\mathrm{max}}$	$C^{\mathrm{Cu-Ni-Al}}_{\mathrm{max}}$
1.17	0.58	0.15	2.13	2.77	2.37

With the proposed 2NN MEAM parameters, MT is reproduced in Cu3Al and CuAlNi. Figures 2 and 3 demonstrate in a 5×5×5 DO3 CuAlNi simulation box, the twinned martensites developed at low temperature after quenching and the austenite recovered when heated, respectively.

CONCLUSIONS

Three new techniques: genetic optimization, matching of elastic constants at finite temperatures, and handling of DO3 reference structure enable a successful and automated process for atomistic potential determination for ternary shape memory alloy CuAlNi. The proposed parameter set in 2NN MEAM reproduces martensitic transformations. With this atomistic potential, dynamics of the thermoelastic MT and stress-induced MT in CuAlNi can be studied.

References

[1] Zhen Y., Chu C.: A deformation-fluctuation hybrid method for fast evaluation of elastic constants with many-body potentials. *Comp. Phys. Commu.* **183**:261-265, 2012.
[2] Plimpton S.: Fast parallel algorithms for short-range molecular dynamics. *J. Comp. Phys.* **117**:1-19, 1995. http://lammps.sandia.gov.
[3] Chipperfield A., et. al.: Genetic algorithm toolbox User's guide. University of Sheffield, UK.
[4] Otsuka K. and Shimizu K.: Morphology and crystallography of thermoelastic Cu-Al-Ni martensite analyzed by the phenomenological theory. *Trans. JIM* **15**:103-108, 1974.