For the meam potential, the total energy E of a system of atoms is given as follows:

$$E = \sum_i \left\{ F_i(\bar{\rho}_i) + \frac{1}{2} \sum_{i \neq j} \emptyset_{ij}(r_{ij}) \right\}, \quad (S1)$$

where F is the embedding energy, which is a function of the atomic electron density ρ *(rho)*, and $\emptyset$ (phi) is a pair potential interaction. The pair interaction is summed over all neighbors J of atom i within the cutoff distance. The relevant parameters of the meam potential are listed in Table S1.

Table S1. The relevant parameters of the Ni–Ni interatomic meam potential.

Type of parameter	Parameter	Type of parameter	Parameter	Type of parameter	Parameter
elt	Ni	*"A" parameter for MEAM*	0.940	*zbl(1,1)*	0
lattice	fcc	*t0*	1.00	*nn2(1,1)*	1
number of nearest neighbors	12	*t1*	3.100	*rho0(1)*	1.000
atomic number	1	*t2*	1.800	*Ec(1,1)*	4.450
atomic weight	58.6900	*t3*	4.360	*re(1,1)*	2.4900
alpha	5.0842	*rozero*	1.000	*alpha(1,1)*	5.0842
b0	2.560	*ibar*	3	*repuls(1,1)*	0.05
b1	1.500	*rc*	4.0	*attrac(1,1)*	0.05
b2	6.000	*delr*	0.1	*Cmin(1,1,1)*	0.81
b3	1.500	*augt1*	0	*Cmax(1,1,1)*	2.80
lattice constant	3.5213	*erose_form*	2		
energy per atom/eV	4.450	*ialloy*	2		

In Table S1, the *alpha, b0, b1, b2, b3, t0, t1, t2,* and *t3* parameters correspond to the standard meam potential parameters in the study of Lee[45]. The *rozero* parameter is an element-dependent density scaling that weights the reference background density and is typically 1.0 for single-element systems. The *ibar* parameter selects the form of the function *G(Gamma)* used to compute the electron density.

The newly developed meam potential[45] more accurately predicted the bulk properties (elastic constants and structural energy differences), point defect properties (vacancy and interstitial formation energy and formation volume, and activation energy of vacancy diffusion), and planar defect properties (stacking fault energy, surface energy, surface relaxation, and reconstruction) of the fcc Ni crystal, and agreed well with relevant experimental information.

The eam/fs potential[46] and eam potential[47] take the same form, and the total energy E_i of an atom i is given as follows:

$$E_i = F_\alpha \left(\sum_{j \neq i} \rho_\beta(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} \emptyset_{\alpha\beta}(r_{ij}), \quad (S2)$$

where F is the embedding energy, which is a function of the atomic electron density $\rho(rho)$; $\emptyset$ *(phi)* is a pair potential interaction; and α and β are the element types of atoms i and j, respectively. The relevant parameters of the eam/fs potential and eam potential are listed in Table S2:

Table S2. The relevant parameters of the Ni–Ni interatomic eam/fs potential and eam potential.

Potential style	eam/fs	eam
atomic number	28	28
mass (g/mol)	58.710	58.710
lattice constant (nm)	0.352	0.352
lattice type	fcc	fcc
N_{rho}	10000	500
d_{rho}	5.0000000E-002	5.01002004008E-04
N_r	10000	500
d_r	4.3171695E-004	9.69696969696E-03
cutoff	4.3171695	4.8000000

In Table S2, N_{rho} and N_r are the number of tabulated values in the subsequent arrays, and d_{rho} and d_r are the spacing in density and distance space for the values in those arrays, respectively.

Both the eam/fs potential[46] and eam potential[47] described well the effects of the defects (point defects, vacancies, interstitial atoms, interface, and other defects) on the evolution of the microstructure of Ni crystal, and the simulation data were in satisfactory agreement with the available experimental results.