Supplementary materials

Molecular Dynamics Study of Friction between Ag Nanoparticle and Two-Dimensional Titanium Carbide Ti2C (MXene)

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Contents:

Description of the interatomic potentials.

1. *Embedded atom method (EAM):*

Within the EAM potential, the total energy of the crystal can be represented as the sum of two terms:

$$U = \frac{1}{2}\sum_{i,j,i\neq j}\varphi(r_{ij}) + \sum_{i}F(\rho_i), \tag{S.1}$$

where $\varphi(r_{ij})$ – pair energy between atoms *i* and *j* separated by distance r_{ij}; $F(\rho_i)$ – embedding energy.

First term in the equation (S.1) has the form:

$$\varphi(r) = \frac{A\cdot\exp\left[-\alpha\left(\frac{r_{ij}}{r_e}-1\right)\right]}{1+\left(\frac{r_{ij}}{r_e}-\kappa\right)^{20}} - \frac{B\cdot\exp\left[-\beta\left(\frac{r_{ij}}{r_e}-1\right)\right]}{1+\left(\frac{r_{ij}}{r_e}-\lambda\right)^{20}}, \tag{S.2}$$

where r_{ij} – distance between atoms *i* and *j*, and r_e, A, B, α, β, κ, λ – parameters of the potential.

Electron density ρ_i is calculated as:

$$\rho_i = \sum_{j,j\neq i} f_j(r_{ij}), \tag{S.3}$$

where electron density function $f_j(r_{ij})$:

$$f_j(r_{ij}) = \frac{f_e \cdot \exp\left[-\beta\left(\frac{r_{ij}}{r_e} - 1\right)\right]}{1 + \left(\frac{r_{ij}}{r_e} - \lambda\right)^{20}}, \tag{S.4}$$

where f_e is a parameter of the potential and all other coefficients are the same as in Eq. (S.2).

Next, the embedding energy $F(\rho_i)$ is calculated according to one of three following equations, depending on the value of ρ_i:

$$F(\rho) = \sum_{i=0}^{3} F_{ni}\left(\frac{\rho_i}{\rho_n} - 1\right)^i, \quad \rho_i < \rho_n, \quad \rho_n = 0.85\rho_e, \tag{S.5}$$

$$F(\rho) = \sum_{i=0}^{3} F_i\left(\frac{\rho_i}{\rho_e} - 1\right)^i, \quad \rho_n \le \rho_i < \rho_0, \quad \rho_0 = 1.15\rho_e, \tag{S.6}$$

$$F(\rho) = F_e\left[1 - \ln\left(\frac{\rho_i}{\rho_e}\right)^\eta\right] \cdot \left(\frac{\rho_i}{\rho_e}\right)^\eta, \quad \rho_0 \le \rho_i \quad . \tag{S.7}$$

where all coefficient, expect ρ_i are parameters of the potential.

Numerical values of all parameters of the EAM potential needed for calculations of expressions (S.1) – (S.7) for different metals are defined in [36] and for Ti and Ag are listed in the table (T1). Full description of the EAM potential and values of its parameters can be found in original work [36].

Table T1. EAM parameters for Ti and Ag [36].

	Ti	Ag
r_e	2.933872	2.891814
f_e	1.863200	1.106232
ρ_e	25.565138	15.539255
α	8.775431	7.944536
β	4.680230	4.237086
A	0.373601	0.266074

B	0.570968	0.386272
k	0.5	0.425351
λ	1.0	0.850703
F_{n0}	–3.203773	–1.729619
F_{n1}	–0.198262	–0.221025
F_{n2}	0.683779	0.541558
F_{n3}	–2.321732	–0.967036
F_0	–3.22	–1.75
F_1	0	0
F_2	0.608587	0.983967
F_3	–0.750710	0.520904
η	0.558572	1.149461
F_e	–3.219176	–1.751274

2. *Two- and three-body potentials:*

The potential energy of the pair interaction is described by the Lennard-Jones potential

$$U_{ij} = 4\varepsilon_0 \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right], \tag{S.8}$$

where r_{ij} – distance between atoms i and j; ε_0, σ – parameters of the potential;

The interaction of three atoms i, j, k, is described by the Axilrod-Teller potential [35]:

$$W_{ijk} = \frac{Z(1+3\cos\theta_i \cos\theta_j \cos\theta_k)}{(r_{ij} r_{ik} r_{jk})^3}, \tag{S.9}$$

where r_{ij}, r_{ik}, r_{jk} – distances between atoms *i-j, i-k*, and *j-k* respectively;

Z – three-body interaction parameter;

$\theta_i, \theta_j, \theta_k$ – angels of the triangle formed by vectors r_{ij}, r_{ik} and r_{jk}.

Numerical values of parameters, used in this study for expressions (S.8) and (S.9) are taken from [30,33,34] and listed in table T2.

Table T2. LJ and AT parameters used in simulations.

	ε_0	σ	Z
Ti-C	0.6	1.8693	
C-C	0.5	2.7031	
Ag-substrate	0.8738×10^{-2}	2.4945	
Ti-Ti-C			60
C-C-Ti			160