MOLECULAR DYNAMICS CALCULATION OF SURFACE TENSION USING THE EMBEDDED ATOM MODEL

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ABSTRACT

Surface tension of liquid iron, gallium, lithium and lead was calculated by the molecular dy-namics method using embedded atom model (EAM) potential. Surfaces were formed by divi-sion of the molecular dynamics model in basic cube into two parts in the external field. Calcu-lated surface tensions for liquid iron at 1823 K, gallium at 303 K, lithium at 463 K and lead at 613 K were 1396, 633, 476 and 308 mJ/m^2 correspondingly. Deviation of calculated values from experimental data was 1-32%.

INTRODUCTION

Molecular dynamics modelling is readily available for calculation of kinetic and potential energies of metals and other materials. In calculation of energy, periodic boundary conditions are used. The energy needed for formation of a surface can be determined by comparing the energy of a system calculated with periodic conditions, with the energy of the system having a free surface.

However, surface energy is defined as the Gibbs free energy change in formation of the unit area of the surface, which calculation is much more challenging. To find the Gibbs free energy of the surface, the reversible work of formation of the surface should be calculated, what re-quires modification of molecular dynamics experiment. A method of reversible formation of the liquid – vacuum interface was suggested by [2]. External field is applied to the equilibrium molecular dynamics model of liquid contained in the basic cube with periodic conditions. This field has a potential $U(x)$ which is presented by Equation (1):

$$U(x) = \lambda\, U_0 \exp\left[- b\,(x - x_m)^2\right] \qquad (1)$$

where x_m is a coordinate of the middle of the basic cube edge aligned along the x axis. The ex-ternal field pushes the particles located at either side of the x=x_m plane in opposite directions. By slowly increasing λ , it is possible to separate the model in basic cube into two parts, with inter-faces located symmetrically with respect to the x=x_m plane. U_o and b in Equation (1) are poten-tial's parameters. In all calculations in this paper U_o is assumed 1 eV.

If the pressure in the model system is maintained at a near zero level, the length of the cube edge should increase proportionally to the width of the gap between the two parts. A model of molten lithium with a gap formed by applying potential (1) is shown in Figure 1 (this work).

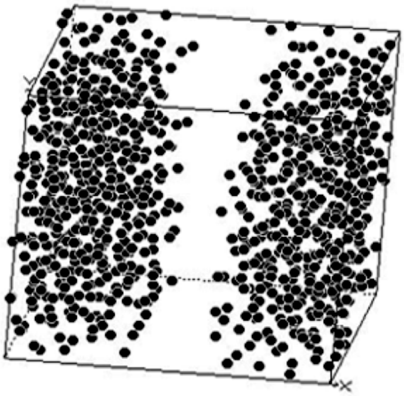

Figure 1: Position of atoms in the model of liquid lithium after formation of a gap (λ = 1016)

It was established [1, 2] that, if the potential energy of the sys-tem can be written as

$$u(r_1, r_2, \ldots r_N) = u_0(r_1, r_2, \ldots r_N) + \lambda u_1(r_1, r_2, \ldots r_N), \qquad (2)$$

where $r_1, r_2, \ldots r_N$ are the radii-vectors of particles 1, 2,...N, and λ is a variable parameter, then the Gibbs free energy of the system, G, will be presented as:

$$(\partial G/\partial \lambda)_{p,T} = \langle U_1 \rangle, \qquad (3)$$

where $<U_1>$ is the average value of the potential $u_1(r_1, r_2, ...r_N)$ for the equilibrium system, which can be calculated in the molecular dynamics experiment [1, 2]. Thus, the Gibbs free energy change in the process of the isobaric–isothermic transition of a sys-tem from the state with a parameter λ_1 to the state with λ_2 is described by Equation (4):

$$\Delta G = G(\lambda 2) - G(\lambda 1) = \int_{\lambda_1}^{\lambda_2} <U_1> d\lambda \tag{4}$$

The integration in (4) should be performed along the isobaric-isothermic route. Equation (4) can also be presented as:

$$\Delta G = G(\lambda_2) - G(\lambda_1) = \int_{\lambda_1}^{\lambda_2} <\lambda U_1> d\ln\lambda \tag{5}$$

This method was applied by Belashchenko and Ostrovski [4] for calculation of surface ten-sion of liquid argon and KCl, for which pair potentials were used to describe interac-tions be-tween particles and potential energy. wCalculated surface tension was in a good agreement with experimental data (deviation was within 2-4%). However, calculation of potential energy of metals based on pair potentials without consideration multi-particle interactions is not appropriate. For example, excess surface energy of amorphous iron, calculated with Pak-Doyama's pair potential was 0.83 J/m^2 [3], while experimental value is much higher, 2.3 J/m^2. Therefore, in calculation of surface tension of metals, multi-particle interac-tions should be taken into account.

In this work, surface tension of liquid Fe, Ga, Li and Pb was calculated using embedded atom model (EAM) to describe multi-particle interactions and potential energy of metals.

MODELLING OF LIQUID IRON AT 1820 K

Modelling of liquid iron was carried out with EAM potential calculated by Belashchenko [5] using experimental diffraction data. The molecular dynamics model with 2048 atoms in the basic cube was constructed at 1820 K using algorithm L. Verlet [12]. The time step was $0.01\tau_0$ (where $\tau_0 = 7.608.10^{-14}$ s is the time unit); the cut-off radius of the EAM potential was set at 8.60 Å.

The reversible division of the system into two parts was performed by applying the external field with potential given by Equation (1). A factor b in Equation (1) was 6.0 Å^{-1}. The system reached equilibrium in a series of runs, 1,000- 5,000 time steps each, after which a number of time steps in each run increased to 20,000. The modelling was performed within the framework of the NpT ensemble; the length of the basic cube edge was adjusted to maintain the pressure in the system at a level close to zero (within 0.1–1.0 MPa).

A model of liquid iron, constructed in the absence of an external field ($\lambda = 0$) at 1820 K, had the density 0.0756 atoms/Å^3 [www.tagen.tohoku.ac.jp]. Then models of liquid iron were con-structed with a parameter λ increasing from zero to 10^{11}. As the λ increased, a planar gap per-pendicular to the x axis aroused at the middle of the basic cube and grew with time. As a result, the total volume and the basic cube edge L increased, while the thickness of the zone occupied by iron atoms decreased.

The mean thickness D of the gap can be calculated from the condition that the liquid is not compressible, therefore the volume occupied by the liquid remains constant:

$$L_0^3 = L^2 (L - D), \tag{6}$$

where L_0 is the length of the basic cube edge in the absence of an external field.
Effect of the intensity of the external field on the characteristics of the model is seen in Table 1. The total energy of the system, H, increased from -6705 eV to -6480 eV when λ increased from zero to 10^{11} The amplitude of fluctuations of the total energy H of the model (the standard deviation) was 7.5–12 eV.

Molecular dynamics simulations yielded the mean energy λU_1 of the system in the external field and the corresponding force $F\lambda$ acting on either half of the system. The value of U_1 at $\lambda = 0$ was determined as the limit of this quantity when $\lambda \rightarrow 0$, where the system was uniform. Fluctuations of λU_1 and F_λ (standard deviations) are also presented in Table 1. Parameters λU_1 and F_λ have maximums at about the same $\lambda = 10^3$.

Table 1: Changes in a model of liquid iron with increasing potential of the external field and formation of a gap. A number of atoms in the model was 2048, temperature 1820 K

λ	L, Å	D, Å	H, eV	λU_1, eV	U_1, eV	$F\lambda$, eV/Å
0	30.045	-	-6705.4	-	-	-
0.01	30.048	-	-6707.4	0.485 ± 0.20	48.49	0.705 ± 0.29
0.02	30.042	-	-6706.1	0.925 ± 0.28	46.27	1.274 ± 0.41
0.05	30.047	-	-6705.6	2.225 ± 0.44	44.50	3.344 ± 0.60
0.1	30.049	0.012	-6705.7	3.948 ± 0.64	39.48	6.269 ± 0.85
0.2	30.050	0.013	-6702.7	6.683 ± 0.82	33.42	11.67 ± 1.20
0.3	30.051	0.018	-6703.9	8.210 ± 0.98	27.37	16.00 ± 1.47
0.5	30.059	0.041	-6703.4	8.924 ± 0.93	17.85	22.34 ± 1.83
1.0	30.047	0.006	-6705.9	8.647 ± 1.09	8.65	27.43 ± 1.95
1.00E+01	30.078	0.098	-6705.8	11.57 ± 1.10	1.16	59.02 ± 2.82
1.00E+02	30.145	0.298	-6687.3	16.87 ± 1.26	0.17	105.0 ± 3.52
1.00E+03	30.284	0.710	-6640.6	17.01 ± 1.31	1.70E-02	122.8 ± 3.92
1.00E+04	30.518	1.396	-6574.6	10.35 ± 1.18	1.04E-03	84.69 ± 3.72
1.00E+06	31.052	2.922	-6505.8	2.190 ± 0.75	2.19E-06	20.87 ± 2.68
1.00E+08	31.826	5.050	-6481.7	0.254 ± 0.46	2.54E-09	2.854 ± 1.75
1.00E+10	31.991	5.488	-6481.4	0.161 ± 0.40	1.61E-11	2.003 ± 1.67
1.00E+11	32.091	5.753	-6480.2	0.137 ± 0.38	1.37E-12	1.966 ± 1.65

Note: L is the length of the basic cube edge, H is the total energy of the system relative to still free atoms without the contribution from the external field, D is the width of the gap between the two halves of the liquid in the basic cube, λU_1 is the energy of the liquid in the external field, and F_λ is the external force acting on the surface.

The surface tension of the model can be found by dividing the Gibbs free energy change calculated using Equation (4) (when $\lambda \leq 1$) and Equation (5) (when $\lambda \geq 1$) by the surface area of two planes $2L^2$.

It is seen in Table 1, that cutting-off the integral at $\lambda = 10^{11}$ is insignificant for the accuracy of calculation. The calculated surface tension of the model of liquid iron at 1820 K is 1396 mJ/m^2. Experimental surface tension at this temperature is equal to 1854 mJ/m^2 [10], which is by 25% higher than the calculated value.

MODELLING OF LIQUID GALLIUM AT 323 K

Molecular dynamics model of liquid gallium was constructed using EAM potential calculated by [6]. The model contained 2997 atoms in the basic cube. As in modelling of liquid iron, the length of the basic cube edge was adjusted to maintain the pres-sure in the system at a zero level. The system was brought about to equilibrium in runs with 1,000-5,000-20,000 time steps; afterwards the external field was applied with a parameter λ varied from zero to 10^9. A parameter b in Equation (1) was 5.0 Å^{-1}. Results of calculation are presented in Table 2.

Total energy of the model increased from -7970 eV to -7858 eV when λ increased from zero to $5.6 \cdot 10^7$ and practically did not changed with further increase in λ. Fluctuation of the total energy (standard deviation) was 1 – 4 eV. Values of λU_1 and F_λ had maximums at $\lambda = 10^4$ and 10^5 cor-respondingly. In the range $3.2 \cdot 10^7 \le \lambda \le 5.6 \cdot 10^7$, force F_λ went down from 37 eV/Å to near zero.

Table 2: Changes in a model of liquid gallium with increasing potential of the external field and formation of a gap. A number of atoms in the model was 2997, temperature 323 K

λ	L, Å	D, Å	H, eV	λU_1, eV	U_1, eV	Fλ, eV/Å
0	38.530	-	-7969.8	-	-	-
0.005	38.532	-	-7969.4	0.295 ± 0.15	59.04	0.392 ± 0.19
0.01	38.530	-	-7969.6	0.547 ± 0.20	54.74	0.739 ± 0.28
0.02	38.530	-	-7969.6	0.987 ± 0.29	49.37	1.482 ± 0.39
0.05	38.533	-	-7969.6	1.659 ± 0.42	33.18	3.000 ± 0.65
0.1	38.529	-	-7969.6	2.047 ± 0.45	20.47	4.417 ± 0.77
0.3	38.530	0.000	-7969.3	2.076 ± 0.47	6.92	6.914 ± 0.90
1.0	38.531	0.004	-7969.7	2.377 ± 0.49	2.38	10.07 ± 1.09
1.00E+01	38.543	0.039	-7969.8	3.573 ± 0.53	0.36	19.51 ± 1.45
1.00E+03	38.541	0.034	-7975.1	8.542 ± 0.67	8.54E-03	59.95 ± 2.11
1.00E+04	38.602	0.216	-7960.6	10.40 ± 0.73	1.04E-03	80.75 ± 2.28
1.00E+05	38.701	0.510	-7933.5	10.30 ± 0.73	1.03E-04	88.36 ± 2.47
1.00E+06	38.795	0.789	-7913.3	7.646 ± 0.70	7.65E-06	71.03 ± 2.47
1.00E+07	38.980	1.335	-7886.4	5.353 ± 0.66	5.35E-07	51.86 ± 2.28
3.16E+07	39.106	1.701	-7873.8	3.703 ± 0.63	1.17E-07	37.04 ± 2.26
5.62E+07	40.552	5.768	-7858.2	3.5E-04 ± 0.05	6.18E-12	7.40E-03 ± 0.21
1.00E+08	40.548	5.758	-7858.5	1.2E-04 ± 0.03	1.24E-12	2.68E-03 ± 0.15
3.16E+08	40.560	5.790	-7858.0	3.7E-04 ± 0.05	1.17E-12	7.75E-03 ± 0.24
1.00E+09	40.547	5.756	-7858.8	2.9E-04 ± 0.04	2.89E-13	6.40E-03 ± 0.19

Calculation of surface tension was done in the same way as for liquid iron. Calculated surface tension of liquid gallium at 323 K was $\sigma = 633$ mJ/m^2, 11% lower than the experimental value 712 mJ/m^2 [10].

MODELLING OF LIQUID LITHIUM AT 463 K

Molecular dynamics modelling of liquid lithium was done with EAM potential calculated by Belashchenko and Ostrovski [7]. A model contained 1968 atoms in the basic cube with the edge length found from the condition of zero pressure. After equilibration of the model at 463 K by molecular dynamics runs with 1000-5000-20000 time steps, the external field was applied with a varied parameter λ in the range 0-10 ^{16}. A parameter *b* in Equation (1) was 5.0 Å^{-1}. Results of calculation are given in Table 3.

Total energy of the model increased from -2973 eV at $\lambda = 0$ to –2854 эВ when λ was 10^{16}. Fluctuation of total energy *H* (standard deviation) was 2 – 3 eV. Values λU_1 И F_λ had maxi-mums at $\lambda = 10^3$ and 10^4 correspondingly. Calculation of surface tension of liquid lithium at 463 K using the same method as described above gave $\sigma = 473$ mJ/m^2 which is very close (within 1%) to the experimental value 468 mJ/m^2 [10].

Table 3: Changes in a model of liquid lithium with increasing potential of the external field and formation of a gap. A number of atoms in the model was 1968, temperature 463 K

λ	L, Å	D, Å	H, eV	λU_1, eV	U_1, eV	$F\lambda$, eV/Å
0	35.311	-	-2973.6	-	-	-
0.01	35.320	-	-2972.6	0.407 ± 0.19	40.72	0.545 ± 0.25
0.02	35.311	-	-2973.5	0.756 ± 0.30	37.79	1.004 ± 0.37
0.03	35.313	-	-2973.1	1.014 ± 0.31	33.80	1.461 ± 0.44
0.05	35.318	0.022	-2973.4	1.395 ± 0.38	27.90	2.306 ± 0.58
0.1	35.312	0.004	-2973.2	1.846 ± 0.51	18.46	3.514 ± 0.66
0.2	35.316	0.015	-2973.1	1.832 ± 0.51	9.16	4.893 ± 0.80
0.3	35.314	0.009	-2973.1	1.853 ± 0.53	6.18	5.674 ± 0.97
0.5	35.319	0.025	-2973.5	1.871 ± 0.49	3.74	6.785 ± 1.05
1.0	35.341	0.090	-2972.1	1.951 ± 0.49	1.95	8.110 ± 1.15
1.00E+01	35.335	0.071	-2973.4	2.886 ± 0.55	0.29	15.36 ± 1.48
1.00E+02	35.405	0.282	-2969.1	4.210 ± 0.60	4.21E-02	26.68 ± 1.78
1.00E+03	35.479	0.502	-2961.4	5.147 ± 0.66	5.15E-03	37.00 ± 2.01
1.00E+04	35.623	0.929	-2947.6	4.908 ± 0.66	4.91E-04	38.63 ± 2.19
1.00E+06	36.015	2.071	-2922.4	3.301 ± 0.62	3.30E-06	30.70 ± 2.14
1.00E+08	36.203	2.609	-2906.6	2.361 ± 0.55	2.36E-08	24.46 ± 2.04
1.00E+10	37.608	6.479	-2861.0	0.369 ± 0.42	3.69E-11	3.971 ± 1.64
1.00E+12	37.844	7.100	-2857.4	0.268 ± 0.38	2.68E-13	3.324 ± 1.54
1.00E+16	38.163	7.933	-2854.3	0.185 ± 0.34	1.85E-17	2.561 ± 1.48

A fragment of the model of liquid lithium at $\lambda = 10^{16}$ is demonstrated in Figure 1. A gap which divides the model to two parts is 7.93 Å wide (see Table 3).

MODELLING OF LIQUID LEAD AT 613 K

EAM potential, used in molecular dynamics modelling of liquid lead was calculated by Belashchenko and Ostrovski [8]. Molecular dynamics model was constructed at 613 K; it con-tained 2997 atoms in the basic cube. Model's equilibrium state was established in runs with 1,000-5,000-20,000 time steps. Afterwards, the external field was applied with a parameter λ (Equation (1)) varied from 0 to 10^{16}. A parameter *b* in Equation (1) was 4.0 Å^{-1}. Calculated results are presented in Table 4.

Increase in parameter λ from 0 to 10^{16} increased total energy from –5468 eV to –5368 eV. Fluc-tuation of total energy of the model (standard deviation) was 3 – 4 eV. Maximums of values of λU_1 and F_λ were at $\lambda = 10^2$ and 10^3 correspondingly. Calculation of surface tension by the method described above for liquid iron gave $\sigma = 308$ mJ/m^2 at 613 K; this value was by 32% lower than the experimental surface tension of liquid lead 454 mJ/m^2 [10].

Table 4: Changes in a model of liquid lead with increasing potential of the external field and formation of a gap. A number of atoms in the model was 2997, temperature 613 K

λ	L, Å	D, Å	H, eV	λU_1, eV	U_1, eV	Fλ, eV/Å
0	45.899	-	-5467.7	-	-	-
0.01	45.899	-	-5467.7	0.538 ± 0.21	53.84	0.628 ± 0.26
0.02	45.899	-	-5467.8	1.026 ± 0.27	51.30	1.223 ± 0.36
0.03	45.897	-	-5468.6	1.457 ± 0.35	48.57	1.764 ± 0.47
0.05	45.895	-	-5468.6	2.092 ± 0.42	41.84	2.775 ± 0.57
0.1	45.895	-	-5468.9	3.017 ± 0.55	30.17	4.807 ± 0.76
0.2	45.902	0.007	-5467.7	3.198 ± 0.64	15.99	7.001 ± 1.00
0.3	45.908	0.027	-5466.7	3.230 ± 0.65	10.77	8.288 ± 1.01
0.5	45.906	0.021	-5467.2	3.105 ± 0.63	6.21	9.626 ± 1.19
1.0	45.911	0.036	-5466.8	3.295 ± 0.61	3.30	11.69 ± 1.25
1.00E+01	45.929	0.089	-5464.9	4.533 ± 0.68	0.45	21.57 ± 1.67
1.00E+02	45.959	0.179	-5460.1	6.045 ± 0.74	0.06	33.48 ± 2.00
1.00E+03	46.070	0.509	-5445.5	5.675 ± 0.74	5.68E-03	36.11 ± 2.17
1.00E+04	46.213	0.934	-5431.4	4.005 ± 0.69	4.01E-04	28.21 ± 2.05
1.00E+06	46.538	1.891	-5408.9	2.030 ± 0.58	2.03E-06	16.78 ± 1.92
1.00E+08	46.827	2.729	-5394.6	1.302 ± 0.52	1.30E-08	12.46 ± 1.80
1.00E+10	47.143	3.635	-5384.2	0.827 ± 0.47	8.27E-11	8.641 ± 1.72
1.00E+12	47.585	4.879	-5374.7	0.400 ± 0.39	4.00E-13	4.402 ± 1.50
1.00E+16	48.133	6.394	-5367.7	0.149 ± 0.31	1.49E-17	1.479 ± 1.13

STRUCTURE OF A MOLECULAR DYNAMICS MODEL IN EXTERNAL FIELD

External field acting in the direction of the basic cube axis x can change the system's structure. A structure of a molecular dynamic model can be characterised by a structure factor $S(K)$, de-fined by Equation (7).

$$S(K) = \frac{1}{N}\left|\sum_{j} \exp\left(\mathrm{i}\,K\,R_j\right)\right|^2 \tag{7}$$

In this equation, R_j is the radius-vector of an atom j, K is the scattering vector, and N is a num-ber of atoms in the model. Ideal crystal has the maximum possible value of $S(\mathbf{K})$ equal to the number of atoms N (in the direction of vectors of inverse lattice), while normal liquids have $S(K)$ values in the range 20 – 30.

To measure $S(K)$ for the molecular dynamic model, the inverse space was scanned changing K with the same step for each projection K_x, K_y, K_z (all together, K had 27,000 different values). In all models, which were subjected to different potentials of the external field (different λ), maxi-mum structure factor was obtained in the direction of the basic cube axis x (100), which was the direction of action of the external force. In any other direction, the structure factor was signifi-cantly less than that in the direction (100).

Table 5 presents structure factors of molecular dynamics models of liquid Fe, Ga, Li, and Pb with different λ for the (100) direction.

Table 5: Maximum values of structure factor S(K) for molecular dynamics models of liquid metals in the direction (1 0 0) in external fields with different potential (different λ)

log λ	Fe	Li	Pb	Ga
-∞ (λ=0)	18.5	17.3	18.5	17.6
-1	22.5	27.5	19.4	57.9
-0.301	38.4	56.2	52.4	96.8
0	48.2	93.6	77.9	163
1	158	152	124	324
2	184	150	208	649
3	161	152	96.3	735
4	70.7	100	45.9	554
5	36.2	72.8	33.8	510
6	31.6	125	68.3	624
7	27.1	96.8	92.2	438
7.50	-	-	-	474
7.75	-	-	-	37.7
8	24.6	126	81.6	35.5
8.50	-	-	-	47.1
9	21.7	96.1	59.7	32.0
10	20.8	21.5	39.2	-
11	26.6	19.1	26.3	-
12	-	22.2	21.8	-
13	-	18.1	20.6	-
16	-	23.1	23.4	-

External field causes a stratification of liquid's structure. Structural factors' maximal values have an order of 10^2; they correspond to the same λ, at which external forces F_λ have a maximum.

Maximal stratification was observed for gallium. Figure 2 shows the model of gallium con-structed at 323 K at λ = 1,000. Stratification includes about 10 atomic layers. At very high λ, the external force F_λ becomes very small, and stratification disappears.

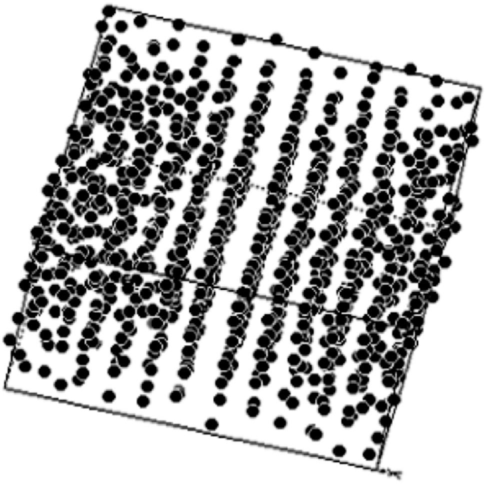

Figure 2: Instantaneous position of atoms in the molecular dynamics model of liquid gallium with N = 2997 and $\lambda = 10^3$. Maximal value of S(K) in the (100) direction is 735

DISCUSSION

Data in Tables 1-4 can be used to find the total energy change ΔU_s caused by formation of two planes on both sides of a gap (without contribution from the external field). The surface internal energy of Fe, Ga, Li and Pb is equal to 1752, 544, 656 И 346 mJ/m^2 correspondingly. As ex-pected, in all cases surface energy is positive.

The entropy of formation of the surface can be found from a relationship $\Delta G_s = \Delta U_s + p\Delta V_s - T\Delta S_s$. Surface entropies, ΔS_s, of Fe, Ga, Li and Pb are equal to 0.196, -0.276, 0.396, 0.062 mJ/m^{2}K respectively. Surface entropies are positive for Fe, Li and Pb and negative for Ga. Cal-culated surface entropies for metals can be compared with surface entropy of liquid argon, which at 90 K was found equal to 0.221 mJ/m^{2}K [4]. Temperature coefficient of surface tension defined as $d\sigma/dT = d\Delta G_s/dT = -\Delta S_s$ is compared with experimental values from [10] below:

$-\Delta S_s$, mJ/m^{2}K	Fe	Ga	Li	Pb
This work	-0.196	0.276	-0.396	-0.062
From	-0.23	-0.088	-0.16	-0.085 [10]

Although significant deviations are observed only for gallium (even the sign of the temperature coefficient is different), calculation of surface entropy from the Gibbs free energy and total en-ergy of the model is not accurate, as ΔG and ΔH have close values. More accurate results for the surface entropy can be expected in direct molecular dynamics modelling at different temperatures.

The use of the multi-particle EAM potential in molecular dynamics modelling gives much better results in calculation of surface tension and surface energy than the use of a pair potential (Pak-Doyama in the case of iron). Departure of calculated surface tension from experimental data was in the range 1-32%. The major reason behind this can be in parameters of the EAM poten-tial which were found using properties of metals at the bulk densities, while density in the sur-face layer decreases down to zero.

Better results can be expected if the model is constructed in the form of a parallelepiped. Then, a gap can be formed without changing the cross-section structure.

CONCLUSIONS

Molecular dynamics modelling of liquid metals with EAM potential gave good results in calcu-lation of surface tension and surface energy of liquid metals. Calculated surface tension for li-quid iron, gallium, lithium and lead near their melting temperature was (mJ/m^2): 1396, 633, 476 and 308 mJ/m^2 correspondingly. These values are lower than experimental surface tensions by 1-32%.

Calculation of surface entropy from total energy and Gibbs free energy is not accurate. It can be improved by constructing thermodynamic models at different temperatures.

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