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MOLECULAR DYNAMICS SIMULATION STUDY OF THERMAL AND MECHANICAL PROPERTIES OF PD, PT AND RH METALS
PD, PT ЖӘНЕ RH МЕТАЛДАРЫНЫҢ ЖЫЛУЛЫҚ ЖӘНЕ МЕХАНИКАЛЫҚ ҚАСИЕТТЕРІН МОЛЕКУЛАЛЫҚ ДИНАМИКА ӘДІСІМЕН ЗЕРТТЕУ
ИССЛЕДОВАНИЕ ТЕПЛОВЫХ И МЕХАНИЧЕСКИХ СВОЙСТВ МЕТАЛЛОВ PD, PT И RH МЕТОДОМ МОЛЕКУЛЯРНОЙ ДИНАМИКИ

Abstract: *The thermal and mechanical properties of Pd, Pt, and Rh pure metals are thoroughly investigated using advanced molecular dynamics (MD) simulations, employing the Sutton-Chen (SC) and quantum Sutton-Chen (Q-SC) potential models. The study aims to analyze the behavior of these metals under increasing temperatures, providing insights into their structural stability and thermodynamic properties. The materials are heated from 0 K to temperatures slightly above their respective melting points in increments of 100 K. Temperature-dependent polynomial and linear functions of the simulation results, derived using both SC and Q-SC models, are obtained to establish a comprehensive understanding of their temperature-dependent properties. Key physical properties, including lattice parameter, density, enthalpy, cohesive energy, elastic constants, bulk modulus, shear modulus, Poisson's ratio, Young's modulus, heat capacity, and thermal expansion coefficient, are systematically calculated. The study compares the performance of SC and Q-SC potentials in predicting these properties and evaluates their accuracy against available experimental and theoretical data in the literature. The findings contribute to a better understanding of the thermomechanical behavior of noble metals, aiding in their potential applications in high-temperature environments and advanced material design. The comparative analysis of SC and Q-SC models also highlights their strengths and limitations in simulating metallic systems.*

Keywords: *Molecular Dynamics; Sutton-Chen potential; Quantum Sutton-Chen potential; transition metals; Mechanical properties.*

Аңдатпа. *Pd, Pt және Rh таза металдарының жылу-механикалық қасиеттері Саттон-Чен (СК) және кванттық Саттон-Чен (Q-SC) әлеуетті модельдерін пайдалана отырып, молекулалық динамиканы (MD) модельдеуді пайдалана отырып зерттеледі. Зерттеу температураның өсуіне қарай осы металдардың мінез-құлқын талдауға бағытталған, бұл олардың құрылымдық тұрақтылығы мен термодинамикалық қасиеттері туралы мағлұмат береді SC және Q-SC модельдерін пайдалана отырып алынған модельдеу нәтижелерінің температураға тәуелді полиномиялық және сызықтық функциялары олардың температураға тәуелді қасиеттерінің толық көрінісін қамтамасыз етеді. Торлы параметрді, тығыздықты, энтальпияны, ұйымшылдық энергиясын, серпімді тұрақтыларды, сусымалы модульді, ширату модулін, Пуассон арақатынасын, Янг модулін, жылу сыйымдылығын, жылу кеңею коэффициентін қоса алғанда, негізгі физикалық қасиеттер жүйелі түрде есептеледі. Зерттеу осы қасиеттерді болжаудағы СК және Q-SC потенциалдарының сипаттамаларын салыстырады және әдебиетте бар эксперименттік-теориялық деректермен салыстырғанда олардың дәлдігін бағалайды. Алынған нәтижелер асыл металдардың термомеханикалық қасиеттерін жақсы түсінуге, олардың жоғары температуралы ортада потенциалды қолданылуына және алдыңғы қатарлы материалдарды әзірлеуге көмектеседі. СК және Q-SC модельдерін салыстырмалы талдау металл жүйелерін модельдеуде олардың күшті және әлсіз жақтарын да бөліп көрсетеді.*

Негізгі сөздер. *Молекулярная динамика, потенциал Sutton-Chen, квантовый потенциал Sutton-Chen, переходные металлы, механические свойства.*

Аннотация. *Термические и механические свойства чистых металлов Pd, Pt и Rh исследуются с помощью моделирования молекулярной динамики (MD) с использованием моделей потенциала Саттона-Чена (SC) и квантового Саттона-Чена (Q-SC). Исследование направлено на анализ поведения этих металлов при повышении температуры, что дает представление об их структурной стабильности и термодинамических свойствах. Материалы нагреваются от 0 К до температур, немного превышающих соответствующие точки плавления с шагом 100 К. Зависящие от температуры полиномиальные и линейные функции результатов моделирования, полученные с использованием моделей SC и Q-SC, позволяют получить полное представление об их температурно-зависимых свойствах. Систематически рассчитываются ключевые физические свойства, включая параметр решетки, плотность, энтальпию, энергию сцепления, упругие константы, объемный модуль, модуль сдвига, коэффициент Пуассона, модуль Юнга, теплоемкость и коэффициент теплового расширения. В исследовании сравниваются характеристики потенциалов SC и Q-SC в прогнозировании этих свойств и оценивается их точность по сравнению с имеющимися экспериментальными и теоретическими данными в литературе. Полученные результаты способствуют лучшему пониманию термомеханических свойств благородных металлов, помогая в их потенциальном применении в высокотемпературных средах и при разработке передовых материалов. Сравнительный анализ моделей SC и Q-SC также подчеркивает их сильные и слабые стороны при моделировании металлических систем.*

Ключевые слова. *Молекулярная динамика, потенциал Саттона-Чена, квантовый потенциал Саттона-Чена, переходные металлы, механические свойства.*

Introduction

Transition metals and their alloys are indispensable for technology. They are used especially in space and micro technologies. Pd, Pt and Rh metals and their alloys are used in many areas such as automotive, space industry and dentistry. Therefore, their study will be useful for technological applications. Parallel to the theoretical and scientific developments, calculational methods based on computer simulations are used very intensively in this field.

Molecular dynamics simulation is used for a time-dependent evaluation of thermodynamic, structural and dynamical properties of metals and alloys [1-6]. The method is also used to calculate interatomic interactions with a correct mathematical function whose gradient gives the forces between atoms. Newton's equations of motion of the system are solved numerically and the system is strained to be in a state of minimum energy, balance point of its phase space [7]. Recently, molecular dynamics computer simulations have started to use empirical many-body potentials to examine the thermodynamic and structural properties of some metals. Usually, the pairwise potential models are used for various model systems. These potentials are insufficient to define metallic bonding. The interatomic interactions that are in real crystalline solids cannot characterized by simple pairwise interactions alone. Cauchy relation between the elastic constants $C_{12}=C_{44}$ is verified by the pure pairwise potential model. This is not the case for the pure metals. Thus, many-body interactions should be taken into account when we study metals and metal alloys. Recent studies have shown that empirical many-body potentials have been developed to include the local density or volume dependence to define metallic binding [8-11]. Among these studies are Daw and Baskes's embedded atom method [12], Finnis and Sinclair's [13,14] empirical many body potentials, the second moment approximation (SMA) to tight binding (TB) model [15], the glue model [16], empirical many body potentials based on Norskovs'effective medium theory [17] and lately the many body potentials developed by Sutton and co-workers[18,19] for fcc transition metals can be listed.

Sutton-Chen potential (SC) has been widely used to examine a range of problems, because this potential has a mathematically simple power law form and a sufficient long-range character. Furthermore, it is suitable for computer modeling. The Sutton-Chen potential is based on the experimental lattice parameter, cohesive energy and bulk modulus [20].

SC potential is reparametrized to develop the temperature dependence of physical properties of fcc metals by fitting the extra physical properties such as phonon frequencies at X point and by taking into account zero point energy (ZPE) [21]. This potential is identified as Quantum Sutton-Chen potential (Q-SC). Quantum Sutton-Chen potential has been used in many scientific research such as glass formations, ranging from alloys, crystallization, surface science problems, clusters,

nanowires, and single crystal plasticity of pure metals to transport properties of fcc transition metals [22-28].

Kart et al. studied the structural properties of Pd, Ag and their alloys. They compared the solidstate properties of Pd and Ag employing SC and Q-SC potential [28]. Kart SO et al. studied the properties of Pd-Ni in liquid and solid phase [9]. They compared some physical properties of mentioned metals and their alloys in the solid and liquid phases by using SC and Q-SC potentials. Although there are many studies for Pd, there is not enaugh work on Pt and Rh by using Q-SC potential. Additionally, Q-SC and SC potentials have not been compared for Pt and Rh.

In this work, we performed molecular dynamics (MD) simulations using the SC and Q-SC empirical many body potentials. We studied temperature dependence of thermal and mechanical properties of Pd, Pt and Rh. Some of our evaluated data on elastic constants, enthalpy and cohesive energy is previously provided by some other outhors [9,10,28] using our method, we reproduced these properties to work out on and to produce new extra data, shear modulus, Poisson ratio, Young's modulus, heat capacity, thermal expansion coefficients and we compared Sutton-Chen and Quantum Sutton-Chen potentials in this study. We compared the calculated simulation results using SC and Q-SC potentials with experimental and theoretical data available in the literature as well.

The article is arranged as follows: SC and Q-SC empirical many body potential models and the method of calculation are defined in Section 2. Section 3 presents the results of computer simulations. These results are compared with the experimental values and other calculations. Finally, conclusions are given in Section 4.

Methodolgy

We have used the Q-SC and SC potentials which are frequently used for FCC transition metals. SC manybody potential is based on the Finnis and Sinclair potential [13]. Empirical manybody Finnis- Sinclair force field includes a repulsive term and an attractive term proportional to square root of the local density. Total potential energy of metals and alloys per atom in a system of N atoms is given by:

$$U_{tot} = \sum_i U_i = \sum_i \left[\sum_{j \neq i} \epsilon_{ij} \frac{1}{2} V(r_{ij}) - c_i \epsilon_{ij} (\rho_i)^{1/2} \right] \qquad (1)$$

$V(r_{ij})$ is a pairwise repulsive term between atoms i and j. Second term describes the manybody cohesive term associated with atom i.

$$V(r_{ij}) = \left(\frac{a_{ij}}{r_{ij}} \right)^{n_{ij}}, \qquad (2)$$

and

$$\rho_i = \sum_{i \neq j} \emptyset(r_{ij}), \qquad (3)$$

$$\emptyset(r_{ij}) = \left(\frac{a_{ij}}{r_{ij}} \right)^{m_{ij}}, \qquad (4)$$

where, r_{ij} is the distance between atoms i and j. a_{ij} is length scale parameter leading to dimensionless arguments for $V(r_{ij})$ and ρ_i. Other parameters (namely c_{ij}, ε_{ij}, n_{ij} and m_{ij}) were obtained by fitting the 0 K properties such as the zero-pressure condition, the cohesive energy and the bulk modulus of the fcc pure metals. c_{ij} is a dimensionless parameter scaling the attractive term. ε_{ij} is an energy parameter obtained from experiment and n_{ij}, m_{ij} are positive integer parameters with n>m. These integer parameters define the range of the two components of the potential. The values of the SC and Q-SC potential parameters for Pd, Pt an Rh are given in Table 1[19, 21].

Table 1. The SC and Q-SC potential parametres for Pd, Pt and Rh pure metals

Metal	Model	N	m	ν(ev)	c	a (A°)
Pd	Q-SC	12	6	0.32864E-2	148.205	3.8813
	SC	12	7	0.41790E-2	108.526	3.8902
Pt	Q-SC	11	7	0.97894E-2	71.336	3.9163
	SC	10	8	1.98350E-2	34.428	3.9200
Rh	Q-SC	13	5	0.24612E-2	305.499	3.7984
	SC	12	6	0.49371E-2	145.658	3.8000

In this study, MD simulations is applied to a super cell consisting of 7x7x7 conventional unit cell (1372 atoms), whose algorithms are based on the extended Hamiltonian formalism [29-33] presented in the studies of Andersen [29], Parinello-Rahman [30], Nosé [31], Hoover [33], and Çağın and Pettitt [32]. The system is made up of a cubic box with 1372 atoms which is sufficient for statistics of the equilibrium properties, such as pressure, temperature, energy, etc. The simulation started with atoms arbitrarily distributed on a fcc lattice subject to the periodic boundary conditions in three dimensions. A 5th-order gear predictor-corrector algorithm is used to integrate equations of motion with the time step of 2 fs. The Parrinello-Rahman piston mass parameter is chosen as W=400 and Nosé-Hoover parameter is set to Q=100. The cutoff distance for the interactions between the atoms is taken to be two lattice parameters to realize maximum capacity and speed of the calculations. However, the temperature effects are taken into account by extending the range by an additional distance of half a lattice parameter. Three successive ensembles are used in simulations. First, HPN (constant-enthalpy and constant-pressure) MD simulation is applied to heat the system and equilibrate at the reached temperatures. The system is heated from 0.1 K to target temperature with increments of 100 K. 2000 time steps are performed for equilibrium of the system, at each temperature. In order to get more accurate values of the melting temperature, the system is heated up with increments of 10 K near to the melting temperature. Afterwards, TPN (constant-pressure and constant-temperature) dynamics are performed to obtain some statistical results such as volume, density and energy of the system. 20000 additional steps are carried out for TPN dynamics. Finally, microcanonical ensemble (EVN) (constant-energy and constant-volume) is used to obtain the elastic constants which are used to compute bulk modulus, shear modulus, poisson ratio and Young's modulus of materials. Where, 50000 additional steps are performed for EVN dynamics. Resultant zero strain averange matrix <h0> are used to obtain pressure dependent properties of the system in EVN dynamics.

Çağın [34,35] derived the fluctuation formula for the calculation of the elastic constant by using the SC potential in the EVN ensemble. The fluctuation Formula is given by

$$C_{\alpha\beta\gamma\kappa} = \frac{\Omega_0}{k_B T}\left(\langle P_{\alpha\beta} P_{\gamma\kappa}\rangle - \langle P_{\alpha\beta}\rangle\langle P_{\gamma\kappa}\rangle\right) + \frac{2Nk_BT}{\Omega_0}\left(\delta_{\alpha\delta}\delta_{\beta\kappa} + \delta_{\alpha\kappa}\delta_{\beta\gamma}\right) + \langle\chi_{\alpha\beta\gamma\kappa}\rangle. \qquad (5)$$

Here angular brackets symbolize the averaging over time and Ω0=deth0 is reference volume for the model system. First term is fluctuation and indicates the contribution from the fluctuation of the microscopic stres tensor Pij. Second term is temperature correction term which represents the kinetic energy contribution and the last term denotes the contribution of the Born term to elastic constants.

The bulk modulus can be determined from

$$B = (C_{11} + 2C_{12})/3 \qquad (6)$$

In addition, shear modulus, Gv, GR and G are calculated from the Voigt-Reuss-Hill arithmetic approximation based on the Voigt and Reuss bounds [43, 44].

$$G_V = \frac{C_{11}-C_{12}+3C_{44}}{5} \quad (7)$$

$$G_R = \frac{5(C_{11}-C_{12})C_{44}}{4C_{44}+3(C_{11}-C_{12})}. \quad (8)$$

The arithmetic average of Voigt and Reuss bounds is called as Voigt-Reuss-Hill approximations

$$G = \frac{G_V+G_R}{2}. \quad (9)$$

Poisson's ratio [39] can be determined from

$$\nu = \frac{C_{12}}{C_{11}+C_{12}}. \quad (10)$$

From the calculated values of the bulk modulus and Poisson's ratio we have also estimated the Young modulus

$$Y = 3B(1-2\nu). \quad (11)$$

Specific heat can be determined from the differential of the enthalpy as follows

$$C_p(T) = \left(\frac{\partial H(T)}{\partial T}\right)_p \quad (12)$$

Thermal expansion coefficient is calculated by using the following relation;

$$\alpha_p(T) = -\frac{1}{a(T)}\left(\frac{\partial a(T)}{\partial T}\right)_p. \quad (13)$$

Results and discussion

Lattice parameter, cohesive energy, enthalpy and density

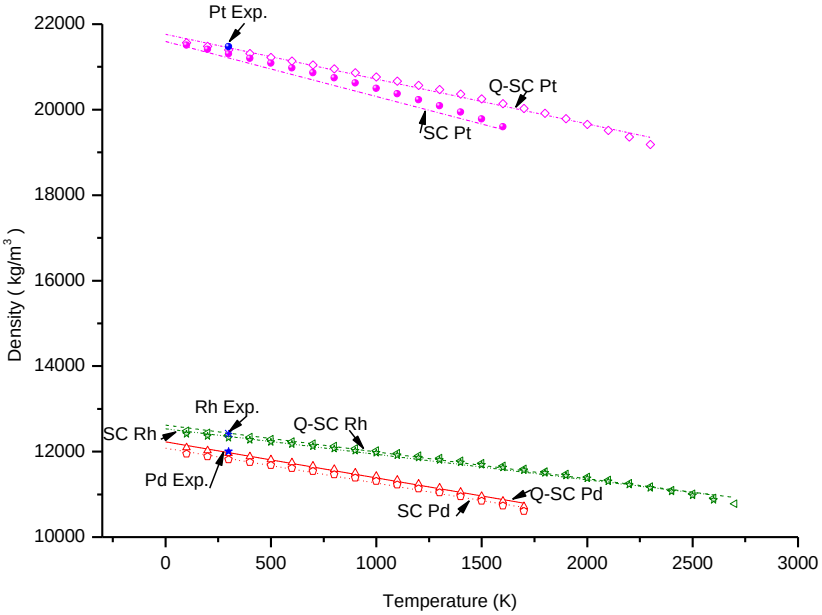
Lattice constant, cohesive energy, density and enthalpy are evaluated in TPN dynamics. The results are given in Table 2. These properties are calculated for both Q-SC and SC potentials.Results are compared to experimental values. The errors found to be very small. The results of Q-SC calculations are in better agreement with the experimental data [36, 37], comparing to SC potential data. For instance, lattice parameter results calculated from Q-SC potential for Pd, Pt and Rh pure metals indicate approximately the deviations of 0.13 %, 0.18 % and 0.16 %, respectively, at 300 K. These deviations are evaluated as 0.54 %, 0.48 % and 0.37 % by SC potential parameters results. Similarly, deviations for density results of Pd, Pt and Rh pure metals calculated from Q-SC potential are 0.69 %, 0.49 % and 0.27 %, respectively, while are being calculated as 1.87 %, 0.92 % and 0.85 % from SC potential at 300 K.

Table 2. Lattice parameter (a), density (ρ), cohesive energy (Ec), enthalpy (H) for Pd, Pt and Rh pure metals calculated from TPN ensemble at different temperatures using Q-SC and SC potential parameters. At each row, the first number gives MD simulation result calculated from Q-SC potentials while the second number gives the SC potentials. The numbers in parantheses are the available experimental value. The experimental density values of Pd and Pt are taken from ref. [36]. The experimental values of density for Rh and experimental lattice parameters are taken from ref. [37].

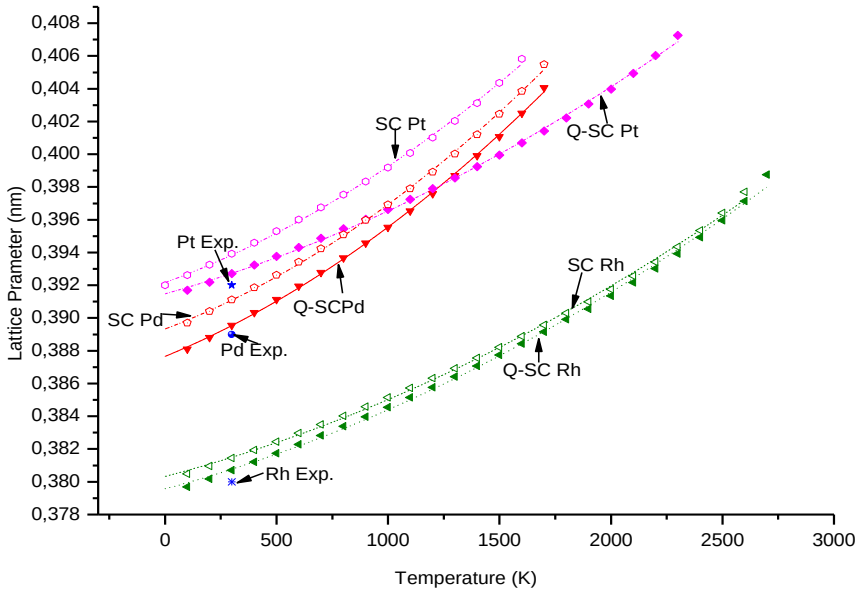
Metals	T (K)	a (Å)	ρ (g/cm3)	H (kJ/mol)	Ec (kJ/mol)
Pd	100	3.880, 3.897	12.091, 11.942 (12.065)	-375.361, -377.618	-375.364, -377.620
	200	3.888, 3.904	12.024,11.878 (12.051)	-372.819, -375.084	-372.822, -375.087
	300	3.895, 3.911 (3.89)	11.955, 11.813 (12.038)	-370.264, -372.523	-370.260, -372.524
	500	3.911, 3.926	11.812, 11.677	-365.008, -367.298	-365.013, -367.298
	700	3.927, 3.942	11.663, 11.535	-359.642, -361.934	-359.645, -361.938
	1000	3.955, 3.969	11.422, 11.303	-351.204, -353.514	-351.212, -353.516
	1200	3.975, 3.989	11.245, 11.133	-345.241, -347.582	-345.247, -347.584
Pt	100	3.916, 3.926	21.561, 21.508	-563.129, -562.921	-563.128, -562.923
	200	3.921, 3.932	21.479, 21.408	-560.625, -560.376	-560.625, -560.375
	300	3.927, 3.939 (3.92)	21.394, 21.303 (21.50)	-558.057, -557.813	-558.057, -557.816
	500	3.937, 3.952	21.222, 21.087	-552.893, -552.611	-552.897, -552.619
	700	3.948, 3.967	21.044, 20.861	-547.647, -547.291	-547.652, -547.293
	1000	3.966, 3.991	20.765, 20.498	-539.595, -538.945	-539.598, -538.953
	1200	3.978, 4.010	20.568, 20.232	-534.053, -533.048	-534.059, -533.060
Rh	100	3.796, 3.804	12.487, 12.408	-555.378, -552.171	-555.378, -552.169
	200	3.801, 3.809	12.437, 12.362	-552.806, -549.642	-552.807, -549.642
	300	3.806, 3.814 (3.80)	12.387, 12.314 (12.42)	-550.228, -547.089	-550.231, -547.090
	500	3.817, 3.824	12.285, 12.217	-545.032, -541.926	-545.038, -541.933
	700	3.828, 3.834	12.181, 12.118	-539.782, -536.702	-539.782, -536.709
	1000	3.845, 3.851	12.018, 11.963	-531.720, -528.672	-531.723, -528.680
	1200	3.857, 3.863	11.904, 11.854	-526.161, -523.159	-526.168, -523.165

In order to present comparison of solid properties which are calculated from Q-SC and SC potential parameters, density, lattice parameter and enthalpy as a function of temperature for Pd, Pt and Rh metals are given in the figs. 1(a), (b) and (c), respectively. When we examine the figures, we see that the curves obtained from Q-SC potential parameters are closer to experimental data than those of SC potential parameters. It can be said that the deviations from experimental values increase parallel to increasing temperature for both SC and Q-SC potentials.

(a)



(b)



(c)

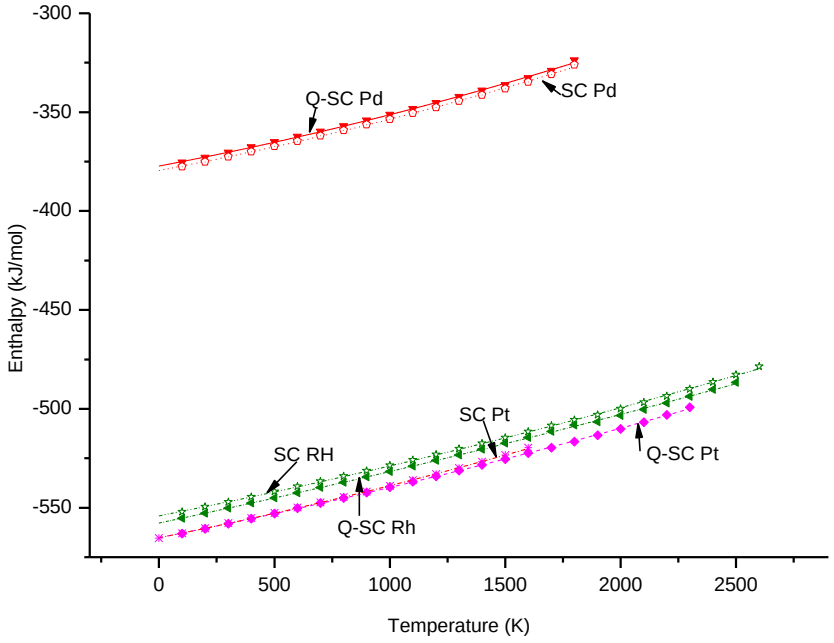


Figure1. (a) Density, (b) lattice parameter and (c) enthalpy of Pd, Pt and Rh pure metals as afunction of temperature for Q-SC and SC potential parameters along with experimental data [36,37].

Specific heat capacity and thermal expansion coefficient

The enthalpy is calculated from the TPN ensemble. The calculated enthalpy results are fitted to a quadratic polynominal using the data below the melting temperature in order to investigate the specific heat capacity as a function of temperature. Fitted data lie between 100 and 1800 K for Pd,

100 and 3000 K for Pt, 100 and 3500 K for Rh. This quadratic polynominal may be chosen as follows:

$$H(T) = a + bT + cT^2 \ (kJ\ mol^{-1}). \qquad (14)$$

Where, T is the temperature. Specific heat capacity can be calculated by taking the first derivative of equation (14). We obtain a, b and c from fitted results of enthalpy data calculated from both Q-SC potential and SC potential parameters at each temperature. The coefficients of thermal expression (a, b and c) in eq. (14), simulated results calculated from Q-SC and SC potantials and experimental data [49] are given in Table 3.

Table 3. Specific heat capacity calculated from both Q-SC potential and SC potential parameters for Pd, Pt and Rh pure metals and coefficients of poliynomial function used to find the heat capacity of metals. Available experimental data [49] are given in the last column at 300 K.

					Cp (kJ mole -1 K-1)	
Metals	A	b x 10-4	c x 10-6	Potential model	Present work	Experiment
Pd	-377.237	220.986	3.849	Q-SC	0.0244084	0.02598
	-379.467	219.023	3.987	SC	0.0242947	
Pt	-565.137	230.903	2.290	Q-SC	0.0244646	0.02586
	-565.171	232.091	3.109	SC	0.0250745	
Rh	-557.727	245.878	1.430	Q-SC	0.0254463	0.02498
	-554.121	231.345	2.110	SC	0.0244006	

When we look at the Table 3, we see that the simulated results and the experimental data given for metals are close to each other. The Q-SC simulated results are in better agreement with experimental data [49] than that of SC simulated ones, except for Pt. For example, heat capacity results calculated from Q-SC potential for Pd, Pt and Rh pure metals indicate approximately to be the deviations of 6.04 %, 5.39 % and 1.86 % respectively, at 300 K. These deviations for SC are calculated approximately to be 6.48 %, 3.03 % and 2.31 %, respectively, at 300 K.
In order to examine the thermal expansion behaviour, we have fitted lattice parameter data below the melting temperature as a function of temperature, to a quadratic polynominal as in heat capacity calculation

$$a(T) = a + bT + cT^2 . \qquad (15)$$

Thermal expansion coefficient can be evaluated by taking the first derivative of equation (15). Table 4 includes the coefficients of Eq. (15), and the simulated results and experimental data at 300 K. Thermal expansion coefficients calculated from Q-SC ve SC potential parametres are more or less similar. But these values are greater than the experimental values [49].

Table 4. Thermal expansion coefficient calculated from both Q-SC potential and SC potential parameters for Pd, Pt and Rh pure metals and coefficients of poliynomial function used to find the thermal expansion coefficient of metals. Available experimental data [49] are given in last column at 300 K.

Metals	a x 10-3	b x 10-8	c x10-11	Potential model	αp x 10-5 (K-1) Present work	Experiment
Pd	387.656	560.125	229.666	Q-SC	1.7916	1.18
	389.332	514.141	245.655	SC	1.6914	
Pt	391.477	380.229	125.834	Q-SC	1.1605	0.88
	392.163	499.900	208.946	SC	1.5873	
Rh	379.566	365.656	117.558	Q-SC	1.1458	0.82
	380.327	356.563	112.639	SC	1.1120	

Elastic constants, bulk modulus, shear modulus and Young's modulus

Elastic constants are calculated by imposing an external strain on the crystal, relaxing any internal parametres to obtain the energy as a function of the strain, and numerically solving for the elastic constants as the curvature of the energy versus strain curve [38]. The elastic constants of solid provide information on the stability and stiffness of materials. The largest contribution to the elastic constants comes from the Born-term in Eq. (5).

In this work, we obtain elastic constants from EVN simulations of 50000 steps for Pd, Pt and Rh pure metals. EVN simulations are performed at temperature between 100 and 2500 K for Pd, 100 and 3000 K for Pt, 100 and 3500 K for Rh depending on their melting points. However, solid state properties are evaluated between 100 K and the melting temperatures. Elastic constants (C11, C12 and C44), bulk modulus (B), Cauchy pressure (C12-C44), Cauchy's ratio (C12/C44), shear modulus (Gv, GR and G), G/B ratio, poisson ratio (ν) and Young's modulus (Y) results are listed in Tables 5, 6 and 7 for Pd, Pt and Rh pure metals, along with experimental and other calculated results. Here, bulk modulus (B), shear modulus (Gv, GR and G), G/B ratio, Cauchy pressure (C12-C44), Cauchy's ratio (C12/C44), poisson ratio (ν) and Young's modulus (Y) are calculated using C11, C12 and C44 elastic constants. The Voigt-Reuss-Hill arithmetic approximation based on the Voigt and Reuss bounds are used for G, ν and Y [43,44].

The calculated elastic constants and bulk modulus are in a good agreement with experiments [36,42] and theoretical studies such as tight-binding (TB), third-neighbor EAM model, long-range FS model, linear augmented plane wave (LAPW) and model pseudopotential (MP) approaches [15,18,38-41].

When we examine Table 5, we see that the elastic constants and bulk modulus calculated from SC potential parameters are closer to the experimental data than those of Q-SC potential parameters, except for C44 of the Pd. C11, C12, C44 and B results calculated from Q-SC potential for Pd show approximately the deviations of 10.6 %, 20.1 %, 13 %, and 10.8 % respectively, at 300 K. These deviations for SC potantial are calculated approximately to be 0.8 %, 6.6 %, 14.2 % and 2.6 %, respectively, at 300 K.

Table 5: Elastic constants C_{11}, C_{12}, and C_{44} (in GPa) calculated from Q-SC and SC potential parametres and Bulk modulus (in GPa), (C_{12}/C_{44}) Canchy's ratio, Cauchy pressure (C_{12}-C_{44}) (in GPa), G_v, G_R and G shear modülüs (in GPa) based on using Voigt-Reuss-Hill arithmetic approximation, (ν) Poisson's ratio and (Y) Young modulus (in GPa) calculated by using elastic constants for Pd pure metal. In the table, some experimental and other theoretically calculated results are also listed for comparison.

				Other theoretical results					
Pd	T (K)	Present work Q-SC	Present work SC	Exp. (36)	(38)	(39)	(15)	(40)	(18)
C_{11}	300	202.806	228.909	227	233	228.7	232	218	248
C_{12}	300	140.587	164.256	176	163	204	178	184	176
C_{44}	300	81.392	82.255	72	63	83.9	73	65	93
B	300	161.327	185.807	181	212	212.8	196	195	200
C_{12}-C_{44}	300	59.194	82.001	-	-	-	-	-	-
C_{12}/C_{44}	300	2.491	2.782	-	-	-	-	-	-
G_V	300	61.279	62.283	-	-	-	-	-	-
G_R	300	49.432	50.843	-	-	-	-	-	-
G	300	55.356	56.563	-	-	11.95	26	17	36
G/B	300	0.3431	0.3044	-	-	-	-	-	-
ν	300	0.4094	0.4177	-	-	0.4724	-	-	-
Y	300	87.691	91.662	-	-	35.19	-	-	-

Table 6, shows that the elastic constants and bulk modulus calculated from SC potential parameters are closer to the experimental values than those of Q-SC potential parameters, except for C11 of the Pt, as discussed in the Table 5. C11, C12, C44 and B results calculated from Q-SC potential for Pt present deviations of 11.2 %, 9 %, 37.7 %, and 8.2 % respectively, at 300 K. These deviations for SC potential are calculated to be 16.1 %, 3.9 %, 14.1 % and 7.2 %, respectively, at 300 K.

Table 6. Elastic constants C_{11}, C_{12}, and C_{44} (in GPa) calculated from Q-SC and SC potential parametres and Bulk modulus (in GPa), (C_{12}/C_{44}) Canchy's ratio, Cauchy pressure (C_{12}-C_{44}) (in GPa), G_v, G_R and G shear modulus (in GPa) based on Voigt-Reuss-Hill arithmetic approximation, (ν) Poisson's ratio and (Y) Young modulus (in GPa) calculated by using elastic constants for Pt pure metal. In the table, some experimental and other theoretically calculated results are also listed for comparison.

				Other theoretical results					
Pt	T (K)	Present work Q-SC	Present work SC	Exp. (36)	(38)	(39)	(15)	(40)	(18)
C_{11}	300	308.092	291.085	347	380	339.9	341	303	314
C_{12}	300	228.392	241.060	251	257	282.1	273	273	258
C_{44}	300	104.692	65.261	76	71	86.5	91	68	74
B	300	254.958	257.735	278	318	301.4	296	283	277
C_{12}-C_{44}	300	123.699	175.799	-	-	-	-	-	-
C_{12}/C_{44}	300	2.942	4.460	-	-	-	-	-	-
G_V	300	78.755	49.161	-	-	-	-	-	-
G_R	300	63.416	39.705	-	-	-	-	-	-
G	300	71.086	44.433	-	-	28.90	34	15	28
G/B	300	0.2788	0.1724	-	-	-	-	-	-
ν	300	0.4257	0.4529	-	-	0.4535	-	-	-
Y	300	113.629	72.6866	-	-	84.01	-	-	-

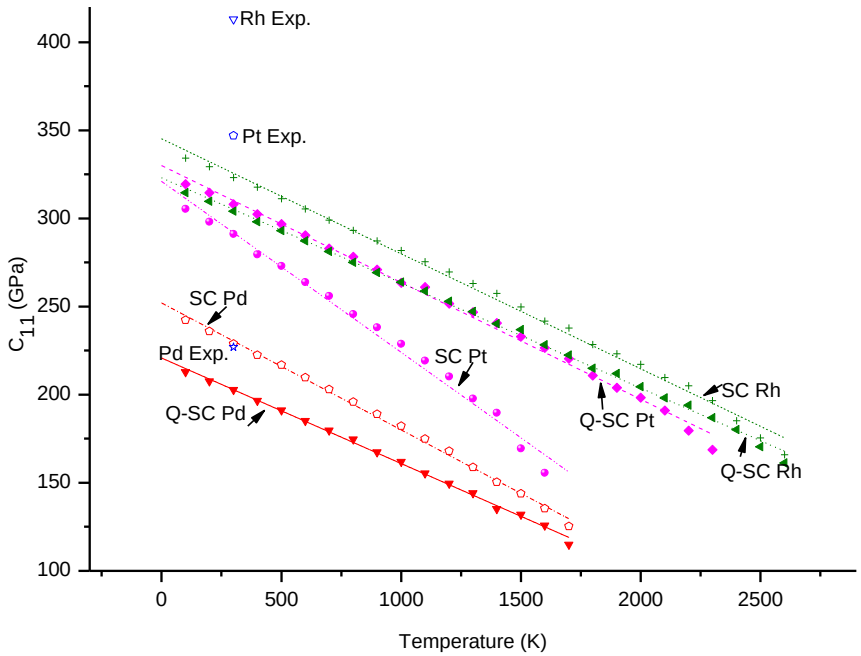
In Table 7, C11,C12, C44 and B results calculated from Q-SC potential for Rh show the deviations of 26.8%, 1%, 25.1%, and 13.3% respectively, at 300 K. These deviations for SC potential are calculated to be 22.2%, 13.1 %, 28.4 % and 5 %, respectively, at 300 K.

Table 7: Elastic constants C_{11}, C_{12}, and C_{44} (in GPa) calculated from Q-SC and SC potential parametres and Bulk modulus (in GPa), (C_{12}/C_{44}) Canchy's ratio, Cauchy pressure (C_{12}-C_{44}) (in GPa), G_v, G_R and G shear modulus (in GPa) based on Voigt-Reuss-Hill arithmetic approximation, (ν) Poisson's ratio and (Y) Young modulus (in GPa) calculated by using elastic constants for Rh pure metal. In the table, some experimental and other theoretically calculated results are also listed for comparison.

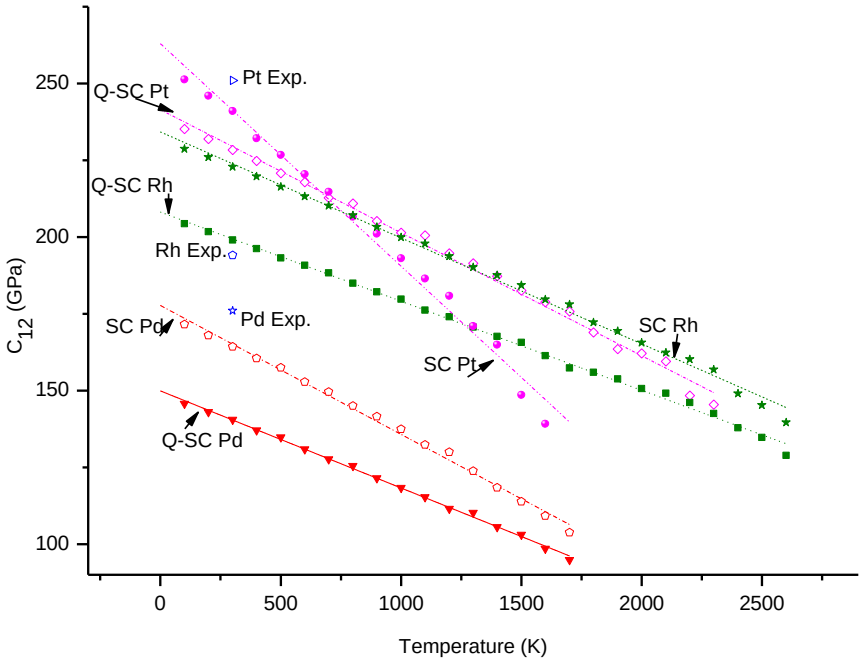
				Other theoretical results					
Rh	T (K)	Present work Q-SC	Present work SC	Exp. (42)	(38)	(15)	(18)	(36)	(41)
C_{11}	300	304.178	323.272	416	491	392	340	413	386
C_{12}	300	198.981	222.855	197	171	237	232	194	171
C_{44}	300	137.738	131.577	184	260	199	143	184	172
B	300	234.047	256.327	270	306	289	269	270	243
C_{12}-C_{44}	300	61.243	91.277	-	-	-	-	-	-
C_{12}/C_{44}	300	2.208	2.456	-	-	-	-	-	-
G_V	300	103.682	99.030	-	-	-	-	-	-
G_R	300	83.605	79.828	-	-	-	-	-	-
G	300	93.643	89.426	-	-	77	54	-	142
G/B	300	0.4001	0.3488	-	-	-	-	-	-
ν	300	0.3954	0.4080	-	-	-	-	-	0.26
Y	300	146.798	141.393	-	-	-	-	-	357

Elastic constants and bulk modulus calculated from Q-SC and SC potential can be compared from figs. 2(a), (b), (c) and (d). When we examine the figures, in general, we see that the curves obtained from SC potential parameters are closer to the experimental data than those of Q-SC potential parameters.

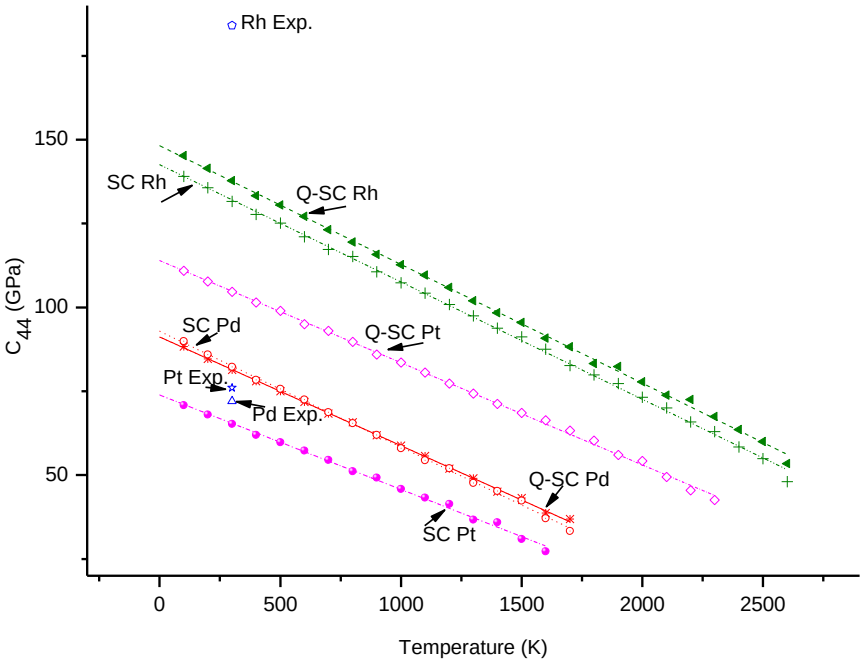
(a)



(b)


Q-SC Pt
Pt Exp.
Q-SC Rh
Rh Exp.
SC Pd
Pd Exp.
SC Rh
SC Pt
Q-SC Pd
C12 (GPa)
Temperature (K)
250
200
150
100
0
500
1000
1500
2000
2500

(c)


Rh Exp.
SC Rh
Q-SC Rh
SC Pd
Q-SC Pt
Pt Exp.
Pd Exp.
Q-SC Pd
SC Pt
C44 (GPa)
Temperature (K)
150
100
50
0
500
1000
1500
2000
2500

(d)

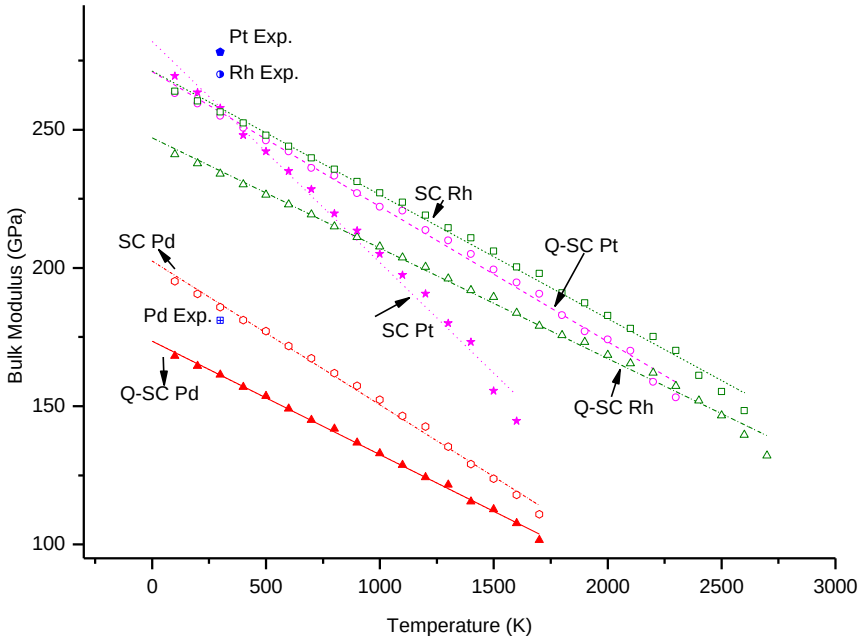


Figure 2. Elastic constants (a) C11, (b) C12 (c) C44 and bulk modulus B of Pd, Pt and Rh pure metals as a function of temperature for Q-SC and SC potential parameters along with experimental data [36,42].

The bulk modulus (B) is described as the measure of average bond strength of materials [41, 45]. It presents a strong correlation with the cohesive energy or the binding energy of the atoms in the crystal. We see that the average atomic bond strength of materials can be determined from the calculated bulk modulus by using elastic constants. The average atomic bond strength of Pd, Pt and Rh pure metals based on the calculated bulk modulus (B) by using Q-SC potential parameters follow the order from large to small as Pt > Rh > Pd. This ordering is, the same for the average atomic bond strength of Pd, Pt and Rh pure metals based on the calculated bulk modulus (B) by using SC potential parameters.

The shear modulus (G) is related with the resistance to plastic deformation while the bulk modulus (B) shows resistant to bond rupture. Therefore, it was reported that the ductile/brittle behaviour of materials could be related empirically to their elastic constants by the ratio of G/B or Poisson's ratio [46, 47]. If G/B >0.5 or ν<1/3, the material is brittle. Otherwise, the material is ductile [45, 46]. It can be said from our study that G/B is smaller than 0.5 and Poisson's ratio is larger than 1/3 for Pd, Pt and Rh pure metals with in both Q-SC and SC potentials. As can be seen from the ratio G/B or Poisson's ratio (ν), all of Pd, Pt and Rh pure metals behave in a ductile manner. Accordingly, ductility of Pd, Pt and Rh pure metals follow the order from large to small as Pt > Pd > Rh. For Cauchy pressure, Pettifor [48] has suggested that it could be used to describe the angular character of atomic bonding in metals and compounds, which reflects the ductile/brittle behaviors of materials. The Cauchy pressure is positive for metallic bonding while it is negative for the directional bonding. The ductile materials show positive Cauchy pressure; otherwise, the material is brittle. If we look to the Cauchy pressure of Pd, Pt and Rh, we see that Cauchy pressure of all of considered metals are positive. These show that Pd, Pt and Rh pure metals are ductile in nature.

Conclusion

In this work, we presented a wide range of properties of Pd, Pt and Rh pure metals. We made comparison between the simulation results obtained by using to Q-SC and SC potential parameters. We compared our results to experimental ones and theoretically calculated values available in literature. The simulation results are closer to the experimental and other theoretical results. Q-SC potential parameters provided fairly accurate temperature-dependent properties at different temperatures.

We analyzed elastic constants C11, C12 and C44 to examine the elastic properties of considered materials. We found bulk modulus (B), Cauchy pressure (C12-C44), Cauchy's ratio (C12/C44), shear modulus (Gv, GR and G) that uses the Voigt-Reuss-Hill arithmetic approximation based on the Voigt and Reuss bounds, G/B ratio, Poisson's ratio (ν) and Young's modulus (Y) results by using elastic constants results.

Examining these results, we can make some comments on the properties of these metals. First, we saw that all of Pd, Pt and Rh pure metals are ductile. Comparing shear modulus, the hardest metal is Rh, middle is Pt and least hard is Pd. Comparing elastic constants, the most plastic is metal is Pt, then Rh and Pd in between them. Comparing cohesive energies, the hardest bounded metal is Pt, then Rh and Pd.

It is seen that MD simulation with SC and Q-SC potential can be used to interpret the technological properties of Pd, Pt and Rh metals.

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