Radiation Physics and Chemistry 149 (2018) 61–64

Contents lists available at ScienceDirect

Radiation Physics and Chemistry

journal homepage: www.elsevier.com/locate/radphyschem

Pressure and temperature dependence of EXAFS Debye-Waller factor of platinum

Nguyen Ba Duc[a,*], Vu Quang Tho[a], Tong Sy Tien[b], Doan Quoc Khoa[c,*], Ho Khac Hieu[c]

[a] *Tan Trao University, Tuyen Quang, Vietnam*
[b] *University of Fire Fighting and Prevention, Hanoi, Vietnam*
[c] *Duy Tan University, Da Nang, Vietnam*

ARTICLE INFO

Keywords:
Anharmonicity
Pressure
Platinum
EXAFS
Debye-Waller factor

ABSTRACT

The anharmonic contributions and pressure effects on extended X-ray absorption fine structure (EXAFS) Debye-Waller factor of platinum metal have been investigated up to 900 K and 14 GPa within the anharmonic correlated Debye model. Parameters of interatomic potential have been derived under the second-moment approximation of tight binding scheme. Our calculations of the EXAFS Debye-Waller factor and anharmonic effective potential are compared with those of experiments showing the good and reasonable agreements. We have shown in detail that the anharmonicity of the thermal vibration of atoms give an important contribution to EXAFS Debye-Waller factor at high temperature. And the increasing of pressure will depress the EXAFS amplitude through the reduction of atomic mean-square relative displacement characterizing the Debye-Waller factor.

1. Introduction

The extended X-ray absorption fine structure (EXAFS) spectroscopy is one of the most powerful technique for investigating local structures around the X-ray absorbing atoms and thermodynamic properties of crystalline as well as amorphous materials (Ozkendir and Yuzer, 2017; Olovsson et al., 2016). The anharmonic EXAFS provides apparently structural and thermodynamic information of substances such as bond distances, coordination number and geometry at various high temperature due to anharmonicity (Rehr, 2000; Iwasawa et al., 2017). This technique can be used independently or in coordination with X-ray diffraction or nuclear magnetic resonance spectroscopy (Ozkendir and Yuzer, 2017). In the recent years, the remarkable developments of EXAFS techniques permit the experiments with unprecedented accuracy under conditions of high pressure and high temperature.

EXAFS oscillation function is often written by means of cumulant expansion approach which contains the second cumulant $\sigma^2 = \sigma^{(2)}$ corresponding to the parallel mean-square relative displacement (MSRD) or EXAFS Debye–Waller factor (DWF) (Bunker, 1983; Fornasini et al., 2001). DWF is an important factor in EXAFS analysis since the thermal lattice vibrations influence sensitively the EXAFS amplitudes through the exponential function $\exp(-2\sigma^2 k^2)$. EXAFS DWF is sensitive to short-range correlations of atomic fluctuations and can be used to examine the anharmonicity effects. There are many methods that have been developed in order to evaluate the temperature effects on EXAFS DWF such as path-integral effective-potential theory (Yokoyama, 1999), statistical moment method (Hung et al., 2010), ratio method (Bunker, 1983), Debye model (Beni and Platzman, 1976) and Einstein model (Frenkel and Rehr, 1993). A simple connection between EXAFS DWF and pair interaction potential has been obtained for a cluster of atoms using the correlated Einstein model (Frenkel and Rehr, 1993) and the first-order thermodynamic perturbation theory (Freund et al., 1991; Yokoyama et al., 1996).

Platinum is a widely used as a standard material for high-pressure experiments and its Hugoniot equation-of state was measured to 660 GPa (Holmes et al., 1989). However, to the best of our knowledge, none of theoretical calculations has been done to predict the temperature and pressure effects on EXAFS DWF of platinum metal. One of the reason is that the Morse potential, which is frequently used in Einstein and Debye model (Holmes et al., 1989; Van Hung and Rehr, 1997), is not suitable to describe the complex atomic interaction of platinum metal. It requires the more accurate interatomic interaction form for metallic systems such as the many body embedded-atom potentials (Daw et al., 1993), Finnis–Sinclair (Finnis and Sinclair, 1984), Rosato–Guillopé–Legrand (Rosato et al., 1989), and Sutton–Chen (Sutton and Chen, 1990; Rafii-Tabar and Sulton, 1991) types. Experimentally, several EXAFS measurements for platinum were performed at ambient pressure (Nishihata et al., 2001) and under pressures up to 6 GPa (Okube et al., 2003).

The purpose of this work is to investigate the anharmonicity

---

* Corresponding authors.
E-mail addresses: ducnb@daihoctantrao.edu.vn (N.B. Duc), khoa_dq@qtttc.edu.vn (D.Q. Khoa).

https://doi.org/10.1016/j.radphyschem.2018.03.017
Received 20 February 2018; Accepted 27 March 2018

contributions and pressure effects on EXAFS DWF. Anharmonic correlated Debye model (ACDM) (Van Hung et al., 2010) has been developed considering pressure effects for platinum crystal on the basis of the interatomic potential which has been derived by the second-moment approximation (SMA) to the tight-binding (TB) model (Cleri and Rosato, 1993). The numerical results will be carried out and compared to other results and experimental values.

2. Theory

In line with the Debye model, Hung et al. developed the ACDM and successfully investigated the temperature-dependent EXAFS cumulants, including DWF (Van Hung et al., 2010). The ACDM in EXAFS is characterized by the anharmonic effective interaction potential $V_{eff}(x)$ where the oscillation of absorber and backscatterer is influenced by their neighbors. The anharmonic effective interaction potential $V_{eff}(x)$ is given by (Van Hung et al., 2010)

$$\begin{aligned} V_{eff}(x) &= V(x) + \sum_{j \neq i} V\left(\frac{\mu}{M_i} x \hat{\mathbf{R}}_{12}.\ \hat{\mathbf{R}}_{ij}\right) \\ &\cong \frac{1}{2} k_{eff} x^2 + k_3 x^3 + \cdots \quad \hat{\mathbf{R}} = \frac{\mathbf{R}}{|\mathbf{R}|}, \end{aligned} \tag{1}$$

here $V(x)$ describes the interaction potential between absorbing and back-scattering atoms; the sum i is over absorber ($i = 1$) and backscatterer ($i = 2$), and the sum j is over all their nearest neighbors, excluding the absorber and backscatterer themselves; k_{eff} is the effective force constant; k_3 is the cubic parameter giving an asymmetry in the pair distribution function due to anharmonicity; and $x = r - r_0$ is the deviation of instantaneous bond length between the two intermediate atoms from equilibrium.

To a good approximation, the second cumulant σ^2 corresponds to the parallel MSRD characterizing EXAFS DWF which has the form in ACDM as

$$\begin{aligned} \sigma^2 &= -\frac{\hbar a_0}{2\pi k_{0eff}} \int_0^{\pi/a_0} \omega(q) \frac{1 + Z(q)}{1 - Z(q)} dq, \\ &= -\sigma_0^2 \int_0^{\pi/a_0} \omega(q) \frac{1 + Z(q)}{1 - Z(q)} dq \quad \text{with} \quad Z(q) = \exp[\beta\hbar\omega(q)], \end{aligned} \tag{2}$$

where a_0 is the lattice constant at temperature T, k_{0eff} is the effective local force constant at ambient pressure which can be derived in terms of interatomic potential parameters, $\sigma_o^2 = \frac{\hbar a_0}{2\pi k_{0eff}}$ is the zero-point contributions to the EXAFS DWF σ^2,$\beta = 1/k_B T$ with k_B is the Boltzmann constant, q is the phonon wave number, $\omega(q)$ is the phonon vibration frequency or the dispersion relation which has the form as

$$\omega(q) = 2\sqrt{\frac{k_{0eff}}{M}} \left| \sin\left(\frac{q a_0}{2}\right) \right|, \quad \left| q \leq \frac{\pi}{a_0} \right|, \tag{3}$$

where M is the mass of composite atoms.

The correlated Debye frequency ω_{0D} and temperature θ_{0D} at ambient pressure can be determined, respectively, as

$$\omega_{0D} = 2\sqrt{\frac{k_{0eff}}{M}}; \quad \theta_{0D} = \frac{\hbar\omega_{0D}}{k_B}. \tag{4}$$

In order to investigate the pressure effects on EXAFS DWF, two parameters in Eq. (2) which should be considered are lattice parameter and local force constant. The volume (and pressure) dependence of lattice constant can be calculated as

$$a = a_0 \left(\frac{V}{V_0}\right)^{1/3} = a_0 \eta^{1/3}, \tag{5}$$

where $\eta = V/V_0$ is the volume compression, V and V_0 are correspondingly the crystal volume at pressure P and zero pressure. The volume dependence of local force constant $k_{eff} = M\omega_D^2/4$ can be estimated by considering the Grüneisen parameter definition in Debye model as

$$\gamma_G = -\frac{\partial \ln \omega_D}{\partial \ln V}, \tag{6}$$

where ω_D is the Debye frequency depending on V(and also pressure P).

At low pressure, the Grüneisen parameter of material can be assumed as constant. However, previous works (Freund et al., 1991; Holmes et al., 1989) showed that the Grüneisen parameter reduced gradually when pressure increased. For platinum metal, Ono and Brodholt (2011) suggested a simple expression of volume-dependent Grüneisen parameter as

$$\gamma_G = \gamma_0 \eta^p, \tag{7}$$

where $\gamma_0 = 2.18(4)$ and $p = 1.75(9)$ (Ono and Brodholt, 2011).

By substituting the Grüneisen parameter γ_G from Eq. (7) into Eq. (6) and taking the integration, we derive the volume-dependent expressions of the Debye frequency ω_D and temperature θ_D, respectively, as

$$\omega_D(\eta) = \omega_{0D} \exp\left[-\frac{\gamma_0}{p}(\eta^p - 1)\right], \tag{8}$$

$$\theta_D(\eta) = \theta_{0D} \exp\left[-\frac{\gamma_0}{p}(\eta^p - 1)\right]. \tag{9}$$

And then we deduce the expression of effective force constant k_{eff} as function of volume compression η as

$$\begin{aligned} k_{eff} &= \frac{M\omega_{0D}^2}{4} \exp\left[-\frac{2\gamma_0}{p}(\eta^p - 1)\right] \\ &= k_{0eff} \exp\left[-\frac{2\gamma_0}{p}(\eta^p - 1)\right], \end{aligned} \tag{10}$$

where $k_{0eff} = M\omega_{0D}^2/4$ is the effective force constant at ambient pressure.

In order to estimate the exact pressure effects on the effective force constant, we need to know a reliable P-V relation or the equation-of-state (EOS) of platinum crystal. There are many EOSs that have been used on studying high-pressure thermo-mechanical properties of materials such as Vinet EOS (Vinet et al., 1987), Birch-Murnaghan EOS (Birch, 1947), Holzapfel EOS (Holzapfel, 1991)… In literature (Cohen et al., 2000), Cohen et al. testified that the Vinet equation would be the most accurate one at high compression. The well-established Vinet EOS has the form as (Cohen et al., 2000)

$$P = 3K_0 \eta^{-2/3}(1 - \eta^{1/3}) \exp\left[\frac{3}{2}(K_0' - 1) \times (1 - \eta^{1/3})\right], \tag{11}$$

where K_0 and K_0' are the isothermal bulk modulus and its first-pressure derivative, respectively.

3. Results and discussion

The expressions derived in the previous section now will be applied to numerically evaluate the temperature and pressure dependences of EXAFS DWF of platinum metal. In this work, we assume the interaction between metallic gold atoms could be described by an empirical many-body potential, derived in analogy of the second-moment approximation of tight binding (TB-SMA) model which is written as (Papanicolaou et al., 1998; Duc et al., 2017)

$$V(r) = V^B(r) + V^R(r), \tag{12}$$

where $V^B(r)$ represents the band-structure term which has a many-body character due to its

square root form as

$$V^B(r) = -\sqrt{\xi^2 e^{-2m[(r/r_0)-1]}}, \tag{13}$$

and $V^R(r)$ is a pair-potential repulsive term (Born-Mayer type),

$$V^R(r) = A e^{-n[(r/r_0)-1]}. \tag{14}$$

It should be noted that, the TB-SMA potential takes into account the essential band character of the metallic bond: the band-structure term is proportional to the effective width of the electronic band and the repulsive pair-potential term, which incorporates the non-band-structure parts, includes electrostatic interactions (Cleri and Rosato, 1993). The potential parameters have typically been determined by fitting to experimental data of cohesive energy, lattice constant, bulk modulus, and elastic constants of the system. The TB-SMA potential parameters determined from first-principles calculations for platinum are respectively $\xi = 2.506$ eV, $A = 0.242$ eV, $m = 3.68$, $n = 11.14$ and $r_0 = 2.68$ Å (Creuze et al., 2008).

Platinum has the structural stability in the face-centered-cubic phase to high pressures. Applying the ACDM for face-centered cubic platinum, the anharmonic interatomic effective potential can be calculated as

$$V_{eff}(x) = V(x) + 2V\left(\frac{x}{2}\right) + 8V\left(-\frac{x}{4}\right) + 8V\left(\frac{x}{4}\right). \qquad (15)$$

Using TB-SMA potential parameters, we derive the effective force constant at ambient pressure as follows $k_{0eff} = 5.26$ eV/Å^2. This second order effective force constant is in reasonable agreement with the measurement of Okube and Yoshiasa (2001) as $k_{0eff} = 5.7$ eV/Å^2. Other value of force constant derived by Okube et al. (2003) at 0.1 MPa is $k_{0eff} = 4.8$ eV/Å^2. In this experiment, Okube et al. (2003) measured the EXAFS spectra near Pt K-edge and L$_3$-edge in the temperature range from 300 to 800 K under pressures up to 6 GPa to investigate the anharmonic thermal vibrations, using large volume high-pressure devices and synchrotron radiation. Furthermore, using the effective force constant derived in our calculations, we deduce the Debye temperature of platinum metal as $\theta_{0D} = 246.68$ K. This value of Debye temperature in our calculations is consistent with previous works which also reported the value for the Debye temperature of platinum around 240 K (Gschneidner, 1964) (Table 1).

Our derived force constants of platinum are used for calculation of the anharmonic effective potential V_{eff} as a function of bond length deviation $x = r - r_0$ as shown in Fig. 1. We also display effective potentials derived by Okube et al. (2003) (under pressure 0.1 MPa) and Okube and Yoshiasa (2001) for comparison. As observed in Fig. 1, there is a small difference between our effective potential and Okube and Yoshiasa' one. The discrepancy of Okube et al.' result could origin from the smaller force constant k_{0eff} and the narrow of potential width under pressure 0.1 MPa in Okube et al.' measurements.

In Fig. 2 we present the temperature dependence of the Debye-Waller factor for the first-shell distances of Pt metal in comparison to those of experimental results (Nishihata et al., 2001; Okube et al., 2003). As seen in this figure the good agreement between theoretical calculations and experimental measurements is found. At low temperature the present ACDM formalism takes into account the quantum-mechanical zero-point vibrations $\sigma_0^2 = 1.3 \times 10^{-3}$ Å^2. When temperature increases the DWF increases rapidly. At $T = 140$ K, the DWF is two times larger than σ_0^2 and at room temperature $T = 300$ K, the DWF is approximately four times larger than σ_0^2. And up to 600 K, DWF has a value 9.9×10^{-3} Å^2 which is more than seven times larger than zero-point vibration contributions. Beyond 150 K, the DWF shows behavior as a linear function of temperature with the slope about 1.6×10^{-5} Å^2/K. Here if we make the fitting our results with quadratic function we derive a small quadratic term as $3.7 \times 10^{-10}\, T^2$ (Å^2).

Table 1

Effective force constant k_{0eff}, Debye frequency ω_{0D} and temperature θ_{0D} of platinum metal at ambient pressure.

	k_{0eff} (eV/Å^2)	ω_{0D} ($\times 10^{13}$ Hz)	θ_{0D} (K)
Present theory	5.26	3.23	246.68
Other works	5.7[a], 4.8[b]	3.14[c]	240[c]

[a] Ref (Okube and Yoshiasa, 2001).

[b] Ref (Okube et al., 2003).

[c] Ref (Gschneidner, 1964).

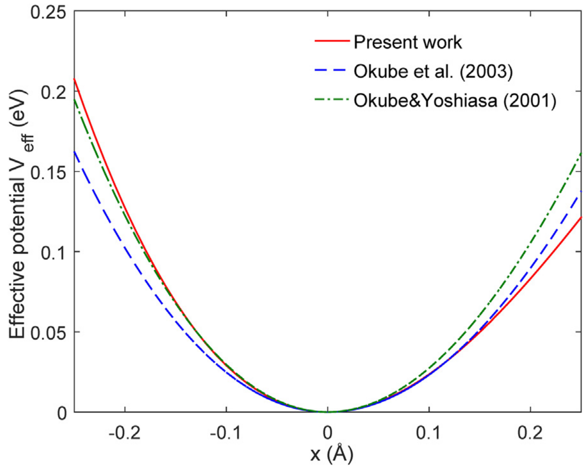

Fig. 1. Anharmonic effective potential of platinum.

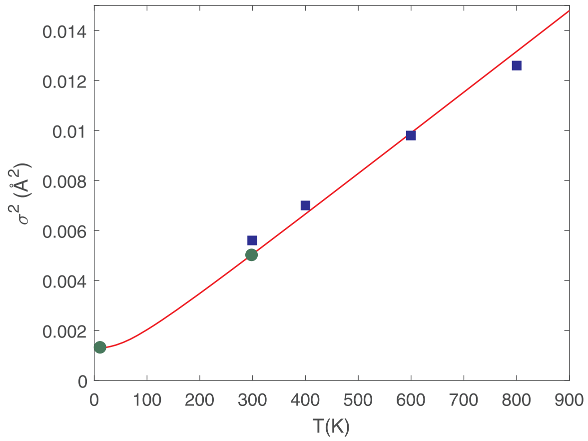

Fig. 2. Temperature dependence of the Debye-Waller factor of platinum. Experimental measurements (solid squares, solid circles) (Nishihata et al., 2001; Okube et al., 2003) are presented for comparison.

Furthermore, it should be noted that the DWF corresponds to the parallel mean-square relative displacement that effects on the amplitudes of EXAFS oscillations. The DWF includes the static disorder σ^2_{static} and dynamic disorder $\sigma^2_{\text{thermal}}$ due to atomic vibrations. The static term σ^2_{static} is the structural disorder or configuration disorder which can be estimated as the quantum-mechanical zero-point vibrations $\sigma_0^2 = 1.3 \times 10^{-3}$ Å^2 for Pt metal. The dynamic term $\sigma^2_{\text{thermal}}$ due to thermal vibrations of atoms or anharmonicity effects of temperature which can be calculated by $\sigma^2_{\text{thermal}}(T) = \sigma^2 - \sigma^2_{\text{static}}$. The contribution of thermal disorder $\sigma^2_{\text{thermal}}$ provides information on the effective bond stretching force constant between absorber-backscatterer pair corresponding to the dynamical properties of them. At room temperature and $T = 600$ K, the thermal disorder contributions have values $\sigma^2_{\text{thermal}}(300\text{ K}) = 3.8 \times 10^{-3}$ Å^2 and $\sigma^2_{\text{thermal}}(600\text{ K}) = 8.6 \times 10^{-3}$ Å^2, respectively. It indicates that the anharmonicity contributions of thermal lattice vibrations become important at high temperature and the present formalism could be used to calculate the DWF of crystals for a wide temperature range.

In order to consider the pressure effects on DWF of platinum, we use the Vinet EOS with the isothermal bulk modulus K_0 and its first-pressure derivative K'_0 are deduced from literature (Ono and Brodholt, 2011). Fig. 3 reports the pressure dependence of the DWF and the difference $\Delta\sigma^2 = \sigma^2(P) - \sigma^2(0\text{ GPa})$ between the DWF at pressure P and

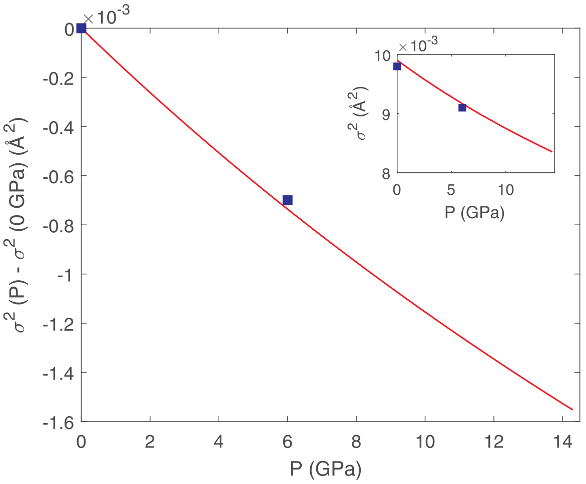

Fig. 3. Pressure dependence of the Debye-Waller factor of platinum. Experimental measurements (solid squares) (Okube et al., 2003) are presented for comparison.

ambient pressure for the first-shell distances of platinum metal in comparison to those of experimental results (Okube et al., 2003). It can be seen in this figure, results of our developed ACDM are in very good agreement with those of Okube et al., measurements up to 6 GPa but with small higher values. The DWF curve of Pt metal diminishes gradually when pressure increases. At zero pressure $P = 0$, the DWF of Pt is 9.9×10^{-3} Å^2. Up to pressure 14 GPa, the DWF σ^2 is reduced and has the value 8.4×10^{-3} Å^2. The slopes of σ^2 curve at zero pressure and at 14 GPa are, respectively, 8.8×10^{-5} Å^2/GPa and 1.36×10^{-5} Å^2/GPa. This result will depress the EXAFS amplitude. This phenomenon can be explained as when pressure increases the vibration of atoms will be limited and it results in the reduction of atomic mean-square relative displacement characterizing the DWF.

4. Conclusions

In this work, we have presented a simple development of ACDM to investigate the temperature and pressure dependences of EXAFS DWF of materials. EXAFS DWF of platinum metal has been calculated numerically up to 900 K and 14 GPa by using the TB-SMA potential. Our calculations have shown that the anharmonicity contributions of thermal lattice vibrations become important to the EXAFS DWF, especially at high temperature. And the increasing of pressure will depress the EXAFS amplitude through the reduction of atomic mean-square relative displacement characterizing the DWF. This approach could be used to verify as well as analyze the future high-temperature and high-pressure EXAFS experiments. It could also be extended to study thermodynamic properties including anharmonicity of alloys in EXAFS theory in the near future.

Acknowledgements

This research is funded by the Tuyen Quang province under grant number ĐT.11-2016.

References

Beni, G., Platzman, P.M., 1976. Temperature and polarization dependence of extended x-ray absorption fine-structure spectra. Phys. Rev. B. 14, 1514–1518.

Birch, F., 1947. Finite elastic strain of cubic crystals. Phys. Rev. 71, 809–824.

Bunker, G., 1983. Application of the ratio method of EXAFS analysis to disordered systems. Nucl. Instrum. Methods Phys. Res. 207, 437–444.

Cleri, F., Rosato, V., 1993. Tight-binding potentials for transition metals and alloys. Phys. Rev. B. 48, 22–33.

Cohen, R.E., Gülseren, O., Hemley, R.J., 2000. Accuracy of equation-of-state formulations. Am. Mineral. 85, 338–344.

Creuze, J., Braems, I., Berthier, F., Mottet, C., Tréglia, G., Legrand, B., 2008. Model of surface segregation driving forces and their coupling. Phys. Rev. B. 78, 75413.

Daw, M.S., Foiles, S.M., Baskes, M.I., 1993. The embedded-atom method: a review of theory and applications. Mater. Sci. Rep. 9, 251–310.

Duc, N.B., Tho, V.Q., Van Hung, N., Khoa, D.Q., Hieu, H.K., 2017. Anharmonic effects of gold in extended X-ray absorption fine structure. Vacuum 145, 272–277.

Finnis, M.W., Sinclair, J.E., 1984. A simple empirical *N* -body potential for transition metals. Philos. Mag. A. 50, 45–55.

Fornasini, P., Monti, F., Sanson, A., 2001. On the cumulant analysis of EXAFS in crystalline solids. J. Synchrotron Radiat. 8, 1214–1220.

Frenkel, A.I., Rehr, J.J., 1993. Thermal expansion and x-ray-absorption fine-structure cumulants. Phys. Rev. B. 48, 585–588.

Freund, J., Ingalls, R., Crozier, E.D., 1991. Extended X-ray-absorption fine-structure study of copper under high pressure. Phys. Rev. B. 43, 9894–9905.

Gschneidner, K.A., 1964. Physical properties and interrelationships of metallic and semimetallic elements. In: Solid State Phys. - Adv. Res. Appl., pp. 275–426.

Holmes, N.C., Moriarty, J.A., Gathers, G.R., Nellis, W.J., 1989. The equation of state of platinum to 660 GPa (6.6 Mbar). J. Appl. Phys. 66, 2962–2967.

Holzapfel, W.B., 1991. Equations of state for ideal and real solids under strong compression. Europhys. Lett. 16, 67–72.

Hung, V.V., Hieu, H.-K., Masuda-Jindo, K., 2010. Study of EXAFS cumulants of crystals by the statistical moment method and anharmonic correlated Einstein model. Comput. Mater. Sci. 49, S214–S217.

Iwasawa, Y., Asakura, K., Tada, M., 2017. XAFS Techniques for Catalysts, Nanomaterials, and Surfaces. Springer International Publishing, Cham.

Nishihata, Y., Mizuki, J., Emura, S., Uruga, T., 2001. EXAFS spectra above Pb and Pt K edges observed at low temperature. J. Synchrotron Radiat. 8, 294–296.

Okube, M., Yoshiasa, A., 2001. Anharmonic effective pair potentials of group VIII and Ib fcc metals. J. Synchrotron Radiat. 8, 937–939.

Okube, M., Yoshiasa, A., Ohtaka, O., Katayama, Y., 2003. Anharmonicity of platinum under Hp and Ht. High. Press. Res. 23, 247–251.

Olovsson, W., Alling, B., Magnuson, M., 2016. Structure and bonding in amorphous $Cr_{1-x}C_x$ nanocomposite thin films: x-ray absorption spectra and first-principles calculations. J. Phys. Chem. C. 120, 12890–12899.

Ono, S., Brodholt, J.P., Price, G. David, 2011. Elastic, thermal and structural properties of platinum. J. Phys. Chem. Solids 72, 169–175.

Ozkendir, O.M., Yuzer, A., 2017. Influence of erbium substitution on the crystal and electronic properties of $FeBO_3$ oxide. Vacuum 141, 222–229.

Papanicolaou, N.I., Kallinteris, G.C., Evangelakis, G.A., Papaconstantopoulos, D.A., Mehl, M.J., 1998. Second-moment interatomic potential for Cu-Au alloys based on total-energy calculations and its application to molecular-dynamics simulations. J. Phys. Condens. Matter 10, 10979.

Rafii-Tabar, H., Sulton, A.P., 1991. Long-range Finnis-Sinclair potentials for f.c.c. metallic alloys. Philos. Mag. Lett. 63, 217–224.

Rehr, J.J., 2000. Theoretical approaches to x-ray absorption fine structure. Rev. Mod. Phys. 72, 621–654.

Rosato, V., Guillope, M., Legrand, B., 1989. Thermodynamical and structural properties of f.c.c. transition metals using a simple tight-binding model. *Philos. Mag. A* 59, 321–336.

Sutton, A.P., Chen, J., 1990. Long-range Finnis–Sinclair potentials. Philos. Mag. Lett. 61, 139–146.

Van Hung, N., Rehr, J., 1997. Anharmonic correlated Einstein-model Debye-Waller factors. Phys. Rev. B. 56, 43–46.

Van Hung, N., Bao Trung, N., Kirchner, B., 2010. Anharmonic correlated Debye model Debye-Waller factors. Phys. B Condens. Matter 405, 2519–2525.

Vinet, P., Ferrante, J., Rose, J.H., Smith, J.R., 1987. Compressibility of solids. J. Geophys. Res. 92, 9319.

Yokoyama, T., 1999. Path-integral effective-potential theory for EXAFS cumulants compared with the second-order perturbation. J. Synchrotron Radiat. 6, 323–325.

Yokoyama, T., Kobayashi, K., Ohta, T., Ugawa, A., 1996. Anharmonic interatomic potentials of diatomic and linear triatomic molecules studied by extended x-ray-absorption fine structure. Phys. Rev. B. 53, 6111–6122.