Melting Temperature of Metals Based on the Nearly Free Electron Model

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We propose a general formula for the melting temperature of metals in terms of electronic mass, electronic number, and nearest-neighbor lattice distance. We derive it from the instability of the transverse phonon in the solid phase, using the nearly free electron model. Including higher order terms of vibrations enhanced near the melting temperature, the electronic restoring force is reduced and the ionic one is negligible. This fact greatly brings down the melting temperature, bringing it close to experimental data in the range of 10 % for Cs, Cu, Au, and Ba. Also, this theory confirms the Lindemann criterion.

KEYWORDS: melting temperature, melting of metals, nearly free electron model, Lindemann criterion

The continuing demand for composite metals to meet wider range characteristics requires a fundamental and more practical method. Among various physical quantities, melting temperature is one of the most fundamental ones. The principal requirement of a theory of melting is to calculate the Gibbs free energies $G_s$ and $G_l$ of the solid and liquid phases as functions of pressure $P$ and temperature $T$. The melting curve in the $P$-$T$ plane is then determined by the condition $G_s(P,T) = G_l(P,T)$, where the calculations of $G_s(P,T)$ and $G_l(P,T)$ are taken as two separate problems. Statistical aspects of melting temperature have received the greatest share of attention. Modern computing techniques have made it possible to compare various approximate schemes with one another and with actual and computer experiments. Most studies have been based on inverse power law, hard-core, or other relatively idealized and short-range forces, such as the Lennard-Jones force field. We cite some of various attempts.

Stroud and Ashcroft studied melting phenomena in Na based on the electron gas model with the electron-ion and electron-electron interactions. They calculated the free energies $G_s$ and $G_l$ of the solid and liquid phases separately and determined the melting temperature by the condition of $G_s = G_l$. After elaborate calculations, they obtained the melting curve which was claimed to be in good agreement with the results of experiments, up to at least 40 kbar in Na. The calculation however is not suitable for other metals except alkali metals, since in the calculation the properties of the free electron were fully taken into account.

Another approach is to determine the melting temperature by the instability of the solid phase. Lindemann investigated the instability condition of the solid phase and proposed a criterion for the melting temperature that the Lindemann ratio $\delta \sim 0.1$ where $\delta$ is the ratio of the mean square amplitude of vibration of each atom about its lattice site to the nearest-neighbor distance of the lattice sites. Using the Lindemann criterion, we can obtain the melting temperature of any crystal. Born calculated the melting temperature from the vanishing point of an elastic stiffness constant $c_{44}$, which means that the instability of the shear vibration in the solid phase occurs at the melting temperature. He confirmed the Lindemann criterion in the solid phase with the Lennard-Jones potential. Fukuyama and Platzman calculated the transverse mode instability point using the self-consistent harmonic approximation (SCHA) as the onset of the superheating transition. They also applied the SCHA to derive Lindemann criterion for the alkali metals and to estimate the melting density and temperature of a Coulomb solid. These theories, however, may not be suitable for metals. Metals are the most plastic solid, and the cohesive energy is mainly a function of density of packing. Local deviations from a strict lattice regularity are easily accommodated. Actually, conduction electrons derive an electronic potential of long-range and oscillating character through the adiabatic principle.

In this paper, we construct a general formula for the melting temperature as the vanishing point of $c_t$, which is the velocity of the transverse phonon in metals. To calculate $c_t$, we use the SCHA for lattice vibrations and the nearly free electron model for conduction electrons. Finally, the melting temperature is given as

$$T_m = 0.145009 \times \frac{\hbar^2 n_e}{m^* R_4^2 k_B}$$

with the Boltzmann constant $k_B$, the Plank constant $\hbar$, the effective mass and the nearest-neighbor lattice distance $R_4$. The parameters $m^*$ and $n_e$ are the effective mass and the number of conduction electrons per site. Except for the numeric factor 0.145009, this equation is on the order of the Fermi temperature $\hbar^2/(m^* R_4^2 k_B) \sim h^2 R_4^2 k_F/(2m^* k_B)$ with the Fermi momentum $h k_F$. The numeric factor is brought by the procedure beyond the harmonic approximation. Note that eq. (1) does not include the ionic mass $M$.

The melting temperatures calculated using eq. (1) agree well with the experimental ones for alkali and noble metals. Moreover, the melting temperatures of various pure and composite metals can be estimated using the parameters as easily accessible experimental data in

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the literature. This theory also deduces the Lindemann ratios of 0.183 and 0.172 for the bcc and fcc lattices, respectively. These values are consistent with the Lindemann criterion.

We proceed to microscopically derive the formula (1) for the melting temperature of metals. Atoms in a metallic material vibrate about their equilibrium positions. We denote the equilibrium position of the atom at the site \( l \) as \( R_l \) and the deviation as \( u_l \). Then, the ionic potential \( V_{\text{ion}} \) is written as

\[
V_{\text{ion}} = \frac{1}{2} \sum_{l,m} v(R_{lm} + u_{lm})
\]

with \( R_{lm} \equiv R_l - R_m \) and \( u_{lm} \equiv u_l - u_m \), where \( v(R_{lm} + u_{lm}) \) is the ionic potential between the atoms at the sites \( l \) and \( m \). In the adiabatic approximation, the one-electron Hamiltonian of the conduction electrons is

\[
H_{\text{el}} = -\frac{\hbar^2}{2m} \nabla^2 + \sum_l w(r - R_l - u_l),
\]

where \( m \) and \( w(r - R_l - u_l) \) stand for the electron mass and the potential of the atom at the site \( l \) with the coordinate \( R_l + u_l \), respectively. The electron field is represented as \( \psi_{\sigma}(r) = \int d^3r \phi_{\sigma}(r) \), where \( \phi_{\sigma}(r) \) is the Wannier function at the site \( l \) and \( a_{\lambda \sigma} \) is the annihilation operator of the conduction electron at the site \( l \) with the spin \( \sigma \). The electronic potential \( V_{\text{el}} \) is written as

\[
V_{\text{el}} = \left\langle \sum_l \int \psi_{\sigma}(r) H_{\text{el}} \psi_{\sigma}(r) dr \right\rangle_{\text{el}} = \frac{1}{2} \sum_{l,m,\sigma} t(R_{lm} + u_{lm}) \left( \langle a_{\lambda \sigma}^* u_{\lambda \sigma} \rangle_{\text{el}} + \text{h.c.} \right),
\]

where \( t(R_{lm} + u_{lm}) = \int \phi_{\sigma}(r) H_{\text{el}} \phi_{\sigma}(r) dr \) is the transfer integral between conduction electrons at the sites \( l \) and \( m \). \( \langle \cdots \rangle_{\text{el}} \) denotes the thermal average over electronic distributions in the ionic configuration \( \{ R_l + u_l \} \). Thus, the Hamiltonian of lattice vibrations is

\[
H = \frac{M}{2} \sum_l \left( \frac{du}{dt} \right)^2 + V_{\text{ion}} + V_{\text{el}}.
\]

In what follows, \( V_{\text{ion}}^{(0)} \) and \( V_{\text{el}}^{(0)} \) respectively denote \( V_{\text{ion}} \) and \( V_{\text{el}} \) with \( u_l = 0 \) for all \( l \) sites, and also their differences are \( \Delta V_{\text{ion}} \equiv V_{\text{ion}} - V_{\text{ion}}^{(0)} \) and \( \Delta V_{\text{el}} \equiv V_{\text{el}} - V_{\text{el}}^{(0)} \). We note that \( \{ R_l \} \) forms the minimum configuration of \( V_{\text{ion}}^{(0)} + V_{\text{el}}^{(0)} \), \( \partial (V_{\text{ion}}^{(0)} + V_{\text{el}}^{(0)}) / \partial R_l = 0 \).

We show how to incorporate nonlinear terms to the restoring force and see how the procedure actually reduces the restoring force. First we calculate \( \Delta V_{\text{ion}} \), which is expanded as

\[
\Delta V_{\text{ion}} = \frac{1}{2} \sum_{l,m} \sum_{\alpha_1, \ldots, \alpha_n} \frac{1}{n!} \partial^\alpha v / \partial R_{l\alpha_1} \cdots \partial R_{l\alpha_n} \times u_{l\alpha_1} \cdots u_{l\alpha_n},
\]

where \( \partial^\alpha v / \partial R_{l\alpha_1} \cdots \partial R_{l\alpha_n} \) is a derivative with \( u_{l\alpha} = 0 \) for all \( l \) and \( m \) sites, and the suffices \( \alpha_1, \ldots, \alpha_n \) denote components. In the SHA, the product \( u_{l\alpha_1} \cdots u_{l\alpha_n} \) is decoupled in pairs. For example, the terms of the same type as \( u_{l\alpha_1}^2 u_{l\alpha_2}^2 u_{l\alpha_3}^2 \) reduce to \( \langle \cdots \rangle \langle \cdots \rangle \langle \cdots \rangle \), where \( \langle \cdots \rangle \) denotes the thermal average over ionic configurations in the equilibrium and the prefactor is the number of combinations for decoupling. Then, we apply the Fourier transformation \( v(R_l) = (1/N_L) \sum_q v(q) e^{i q R_l} \) with \( N_L \), which is the number of lattice sites. Thus, \( \Delta V_{\text{ion}} \) is written as

\[
\Delta V_{\text{ion}} = \frac{1}{4N_L} \sum_q v(q) \sum_{l,m} \langle \alpha \cdot \alpha \rangle u_{l\alpha m}^* u_{l\alpha m} e^{i q (R_l - R_m)}.
\]

The nonlinear terms have been incorporated into the exponential factor \( \exp[-\langle \langle q \cdot u \rangle \rangle^2 / 2] \) that reduces \( \Delta V_{\text{ion}} \). Here, we introduce a common reduction factor \( \exp[-\langle \langle q \cdot u \rangle \rangle^2 / 2] \), where \( u \) is the displacement between the nearest-neighbor sites, since the nearest-neighbor terms are dominant. Defining the effective interaction \( v(q) = v(q) \exp[-\langle \langle q \cdot u \rangle \rangle^2 / 2] \), we obtain

\[
\Delta V_{\text{ion}} = \frac{1}{4N_L} \sum_q v(q) \sum_{l,m} \langle \alpha \cdot \alpha \rangle u_{l\alpha m}^* u_{l\alpha m} e^{i q (R_l - R_m)}.
\]

We apply the Fourier transformation to the displacement as \( u_l = \sum_q u_q e^{i q R_l} \). The coefficient \( u_q \) is written as

\[
u_q = \sum_{\lambda \sigma} u_{q \lambda} e_{\lambda \sigma}
\]

with \( \lambda = 1 \) and one of the transverse modes by \( \lambda = \tau \). Then, eq. (8) is written as

\[
\Delta V_{\text{ion}} = \frac{1}{2} \sum_{q, \lambda} u_{q \lambda} u_{-q \lambda} A_{\lambda}(G, q)
\]

with \( A_{\lambda}(G, q) = \bar{v}(G+q)((G+q) \cdot e_{\lambda \sigma})^2 - \bar{v}(G)(G \cdot e_{\lambda \sigma})^2 \), where \( G \) stands for the reciprocal lattice vector.

Next, we calculate \( \Delta V_{\text{el}} \). The change in ionic configuration from \( \{ R_l \} \) to \( \{ R_l + u_l \} \) changes the potential in eq. (3) by \( \delta w = w(r - R_l - u_l) - w(r - R_l) \). Accordingly, the transfer integral changes by \( \delta t(u_{lm}) = t(R_l + u_l) - t(R_l) \), which is on the same order as \( \delta w \). The average of the electron operators in eq. (4) changes as

\[
\langle a_{\lambda \sigma}^* u_{\lambda \sigma} \rangle_{\text{el}} = \langle a_{\lambda \sigma}^* u_{\lambda \sigma} \rangle_{\text{el}} + O((\delta w / \epsilon_F)^2),
\]

where \( \langle \cdots \rangle_{\text{el}} \) is the thermal average for \( \{ R_l \} \) and \( \epsilon_F \) is the Fermi energy. Then, we obtain \( \Delta V_{\text{el}} = (1/2) \sum_{l,m,\sigma} \delta t(u_{lm}) \langle \langle \sigma \rangle \rangle \langle \sigma \rangle_{\text{el}} + \text{h.c.} \) in the first order of \( \delta w / \epsilon_F \) as an approximation. We manipulate \( \Delta V_{\text{el}} \) in the same manner as that for \( V_{\text{ion}} \). Using the Fourier transform, \( a_{\lambda \sigma} = (1/\sqrt{N_L}) \sum_k a_{k \lambda \sigma} e^{i k R_l} \), \( t(R_l) = (1/N_L) \sum_k t(k) e^{i k R_l} \), and \( \hat{f}(k) = t(k) \hat{f}(k \cdot e_{\lambda \sigma})^2 \), we obtain

\[
\Delta V_{\text{el}} = \frac{1}{2N_L} \sum_{q, \lambda} u_{q \lambda} u_{-q \lambda} \sum_{k, \sigma} f(k)(k \cdot e_{\lambda \sigma})^2
\]

with \( B_{\lambda}(k, q) = \hat{f}(k + q)((k + q) \cdot e_{\lambda \sigma})^2 - \hat{f}(k)(k \cdot e_{\lambda \sigma})^2 \).

Using eqs. (9) and (10), the Hamiltonian (5) exhibits a bilinear form. Hence, the energy \( \omega_{q \lambda} \) of the normal
vibration exhibits the dispersion

\[ M c_{q\lambda}^2 = \sum_G A \lambda(G, q) + 2 \frac{2}{N_L} \sum_k f_k B \lambda(k, q). \]  

(11)

The longitudinal velocity \( c_{ql} \) and transverse velocity \( c_{qT} \) are determined using \( \omega_{ql} = c_{ql} |(\mathbf{e}_{ql} \parallel q) \) and \( \omega_{qT} = c_{qT} |(\mathbf{e}_{qT} \perp q) \) for a small momentum \( q \), respectively. Then, the longitudinal velocity is given as

\[ M c_{qT}^2 = v(0) + \sum_{G \neq 0} \Gamma_q(G) \bar{v}(G) + 2 \frac{2}{N_L} \sum_k f_k \Gamma_q(k) \bar{t}(k) \]  

(12)

with the operator \( \Gamma_q(K) = 1 + 2(e_{ql} \cdot K)(e_{qT} \cdot \nabla K) + (1/2)(e_{ql} \cdot K)^2(e_{qT} \cdot \nabla K)^2 \) for \( K = G \) or \( k \). The transverse velocity is given as

\[ M c_{qT}^2 = \sum_{G \neq 0} \Gamma_q(G) \bar{v}(G) + 2 \frac{2}{N_L} \sum_k f_k \Gamma_q(k) \bar{t}(k) \]  

(13)

with the operator \( \Gamma_q(K) = (1/2)(e_{ql} \cdot K)^2(e_{qT} \cdot \nabla K)^2 \) for \( K = G \) or \( k \). In the limit of \( q \to 0 \), we simply denote the velocities as \( c_1 \) and \( c_t \). The velocities depend on the renormalized ionic potential \( \bar{v} \) and the transfer integral \( \bar{t} \), which include \( c_1 \) and \( c_t \) in reduction factors. Hence, we obtained a set of self-consistent equations (12) and (13) to determine \( c_1 \) and \( c_t \) as functions of temperature. As temperature increases, \( \bar{v} \) and \( \bar{t} \) decrease and then \( c_1 \) and \( c_t \) decrease. We find that \( c_1 \) vanishes at a special temperature, which we identify the melting temperature. On the other hand, the longitudinal velocity \( c_1 \) remains finite because eq. (12) includes the ionic potential \( v(0) \), which is independent of temperature. Actually, the longitudinal phonon remains in the liquid phase.

We show that near the melting point, the ionic potential \( \bar{v}(G) \) for \( G \neq 0 \) becomes much smaller than the transfer integral \( \bar{t}(k) \) for sc, bcc and fcc crystals. The Fourier transforms of the ionic potential \( \bar{v}(G) \) and the transfer energy \( \bar{t}(k) \) are given as

\[ \bar{v}(G) = v(G)(e^{-|G|u_4}) = v(G)e^{-\frac{1}{2}|G|^2u_4^2}, \]  

(14)

\[ \bar{t}(k) = t(k)(e^{-ik_4u_4}) = t(k)e^{-\frac{1}{2}k_4^2u_4^2}. \]  

(15)

Here, the mean square amplitude of the vibration between the neighboring sites is calculated as

\[ \langle u_4^2 \rangle = \sum_q \left( 2 \sin \frac{q \cdot R_4}{2} \right)^2 \langle u_4 u_{-4} \rangle, \]  

(16)

where \( R_4 \) is the nearest-neighbor lattice coordinate and the last factor is calculated as

\[ \langle u_4 u_{-4} \rangle = \frac{1}{N_L} \left\{ \frac{2}{c_1} g \left( \frac{c_4 q}{k_B T} \right) + \frac{1}{c_q} g \left( \frac{c_4 q}{k_B T} \right) \right\} \]

with the function \( g(x) = (e^x - 1)^{-1} + 1/2. \) At high temperatures, eq. (16) reduces to

\[ \langle u_4^2 \rangle = \frac{k_B T R_4^2}{3M} \left( \frac{2}{c_4^T} + \frac{1}{c_4} \right) \]  

(17)

on the assumption of \( c_4 q / k_B T \ll 1 \). We compare two reduction factors in eqs. (14) and (15). We take the magnitude \( G_{\text{min}} \) of one of the smallest reciprocal lattice vectors for the lower bound of \( |G| \) in eq. (14) and

The Fermi wave number \( k_F \) for the upper bound of \( |k| \) in eq. (15). Then, the ratio \( r(t) = G_{\text{min}}^2 / |k| \) measures the relative importance of \( \bar{v}(G) \) against \( \bar{t}(k) \), where \( n_e \) is the electron number per site. For a simple cubic lattice, the ratio is written as \( r(t) = (8\pi/3n_e)^{2/3} \), which gives \( r(1) = 4.12 \) and \( r(2) = 2.60 \). For a bcc lattice, the ratio is written as \( r(t) = 2(4\pi/3n_e)^{2/3} \), which gives \( r(1) = 5.20 \) and \( r(2) = 3.28 \). For an fcc lattice, the ratio is written as \( r(t) = 3(2\pi/3n_e)^{2/3} \), which gives \( r(1) = 4.91 \) and \( r(2) = 3.09 \). These estimations show that \( \bar{v}(G) \) becomes negligible in comparison with \( \bar{t}(k) \). Therefore, near the melting point, we reasonably drop the first term in eq. (13) and obtain

\[ c_{qT}^2 = \frac{1}{MN_L} \sum_k f_k \left\{ (k \cdot e_{qT})^2 (e_{qT} \cdot \nabla_k)^2 \bar{t}(k) \right\}. \]  

(18)

This equation implies that the melting temperature is determined solely by the force constant given by the attractive potential due to conduction electrons.

Since we have used the nearly free electron model, we have \( \bar{t}(k) = h^2 k^2/(2m^*) \) with the effective electron mass \( m^* \). When the sound propagates along the \( x \)-direction with the polarization vector parallel to the \( y \)-direction, eq. (18) becomes

\[ c_{qT}^2 = \frac{V}{(2\pi)^3 MN_L} \int f_k k_y^2 \frac{\partial^2}{\partial k_x^2} \left( \frac{h^2 k_x^2}{2m^*} e^{-\kappa k^2} \right) d^3k \]  

(19)

with \( \kappa = k_F^2 / (9MN_L^2) \) under the assumption of \( c_0 \ll c_1 \). By defining the constants \( T_0 = 9h^2 n_e/(10m^* R_4^2 k_B) \) and \( c_0 = h k_F n_e^{1/2} / (10 M M^*)^{1/2} \) and introducing the scaled variables \( \gamma = c_2^2 / c_{10}^2 \) and \( \tau = T / T_0 \), eq. (19) reduces to

\[ \gamma = \left( 1 - \frac{\tau}{\tau_0} \right) e^{-\tau/\gamma} \]  

(20)

after integration. Note that this relation is universal, and in particular, \( M \) is absorbed in the scaled velocity \( \sqrt{\gamma} \).

By introducing a variable \( x = \tau / \gamma \), eq. (20) is written as \( \gamma = x(1 - x) e^{-x} \). The maximum \( \tau, \tau_m \), is determined by \( d\tau / dx = 0 \). We denote \( x \) and \( \gamma \) for \( \tau = \tau_m \) as \( x_m \) and \( \gamma_m \).
\[\delta^2 = \left(\frac{\langle u_0^2 \rangle}{R_d^2}\right)^2 \sim \frac{\alpha k_B T_m}{M} = \frac{\alpha}{R_d^2} \left(\frac{k_B R_d}{\sqrt{\varepsilon_m}}\right)^2.\] (23)

With \(\alpha R_d^2 = 0.05529\) (bcc) and 0.05224 (fcc), and with \(18/(k_B R_d)^2 = 1.580\) (bcc) and 1.493 (fcc), we obtain
\[\delta = 0.183\] (bcc) and 0.172 (fcc). (24)

These values are consistent with and then confirm the Lindemann criterion \(\delta \sim 0.1\). Our results also agree with \(\delta \approx 0.15\) and 0.126 obtained by numerical calculations with the soft core repulsive potential \(r^{-n}\) (\(n > 3\)) and the hard core repulsive potential, respectively.\(^{18,23}\)

In summary, we use the shear instability of the solid phase to derive the equation for the melting temperature. We renormalize the ionic and electronic restoring forces, including higher order terms of displacement enhanced near the melting temperature by applying SCHA. The total force due to the renormalized ionic potential \(\bar{v}(\mathbf{G})\) with \(\mathbf{G} \neq 0\) decreases significantly and becomes negligible near the melting temperature. Hence, the velocity \(\gamma_i\) is solely determined by the force via conduction electrons. We obtain the melting temperature from the vanishing point of velocity \(\gamma_i\) without any adjustable parameters. The theoretical melting temperature \(T_m^{(th)}\) is consistent with the experimental one \(T_m^{(ex)}\). We can estimate the melting temperatures of various pure and composite metals if we have the values of \(m^*, R_d\) and \(n_e\). The Lindemann criterion is obeyed. Finally, we discuss melting temperatures of the transition, lanthanide, and actinide metals. Using the experimental data of \(R_d\), we obtain \(T_m^{(th)}/T_m^{(ex)} = A(n_e/m^*)^2\): \(A = 0.17\sim 0.12\) (3d), \(0.6\sim 0.9\) (4d), and \(0.8\sim 0.5\) (5d) for the transition metals; \(A = 0.7\sim 0.9\) for the lanthanide metals; and \(A = 0.5\sim 0.7\) (Th, Pa, and Am) for the actinide metals. If \(n_e/m^*\) is about 1, \(T_m^{(th)} / T_m^{(ex)} \sim 1\). Actually, \(n_e/m^* \sim 2\) in the lanthanide and actinide metals, and the transition metals may share similar values.

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