



## Surface tension of liquid transition and noble metals



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### ABSTRACT

We have studied the surface tension of all liquid transition and noble metals using extended Mayer's empirical formula. For interionic interaction in metals, Bretonnet and Silbert (BS) pseudopotentials and the embedded atom method (EAM) potentials are chosen. Self-consistent variational modified hypernetted chain (VMHNC) integral equation theory is used to describe liquid state. The premier ingredients of the extended Mayer's formula are the effective hard sphere (HS) diameter and packing fraction. We calculated HS diameter using both BS and EAM potentials in conjunction with the VMHNC theory. We have found that the surface tension obtained using EAM potentials are in very good agreement with the available experimental data.

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### 1. Introduction

The knowledge of surface properties of condensed matters have attracted scientists, metallurgists and technologists from the long past to the present decade for their multiple applications, such as soldering, brazing, sintering and dying [1–18]. Surface properties, for example, surface tension are a dominating factor for the phenomena such as gas absorption, nucleation of gas bubbles, nucleation and growth of non-metallic inclusions and slag or metal reactions [19]. The knowledge of physics at the liquid surface therefore is necessary to understand such processes. The surface properties of a liquid metal are greatly influenced by its structural and thermodynamical properties [17,18]. Thus a theory is required which can explain the liquid structure and thermodynamics of the system accurately.

The surface properties can be studied using both different theories, for example, the statistical mechanical theory [1–6], density functional theory [8,9] and computer simulation method [12,13] and various experimental techniques, for example, sessile drop method [20], levitated drop method [21,22], oscillation drop technique [23], drop-weight method [20,24], etc. The statistical mechanical theory involving surface tension and intermolecular forces goes back to Fowler [3]. This theory was subsequently analyzed and improved by different authors [6,9,10]. The author in [10] derived an expression for the surface tension by describing the interionic interaction within the pseudopotential approach but faced difficulties while

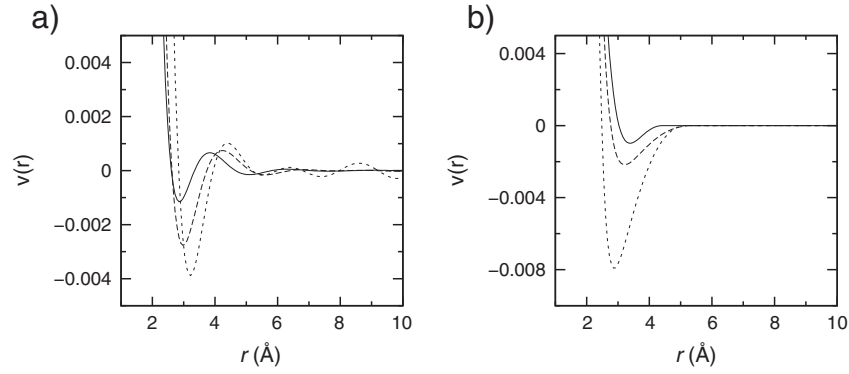
applying it to liquid transition metals because of the strong electron–ion interaction in transition metals. On the other hand, Fowler's formula failed to provide precise values of surface tension if the potential has a long Friedel type oscillating tail. It is, therefore, necessary to cut the integrand up to a certain interionic distance. It is noted that Korkmaz and Korkmaz [17,18] have applied Fowler's formula and calculated the surface tension for a few liquid transition metals using the individual version of local pseudopotential proposed by Fiolhais et al. [25,26]. In their calculation, the effective interionic interaction was taken up to interionic distance,  $r = 41 \text{ \AA}$ . About two decades ago, Egry et al. [14] derived a relation between surface tension and viscosity and then estimated them near melting points for a few liquid transition and noble metals. Recently, Yokoyama et al. [15] have also presented an empirical formula which connects surface tension to the diffusion coefficients and hard sphere (HS) diameter. The problem in Refs. [14,15] is that surface tension depends on the transport coefficients of the transition metals which are very difficult to measure experimentally [17,18,27]. To overcome the above limitations, a simpler relation is required.

Using a scaled-particle theory [20], Mayer proposed a relation between isothermal compressibility and surface tension [28]. Following Meyer, recently, Blairs [29] applied this relation to estimate sound velocities of transition, rare earth and actinide elements at the melting point but still surface properties, especially surface tension, remained un-explored. Therefore, in the present study, we have, firstly, derived a suitable relation for the surface tension from Mayer's formula in terms of HS diameter and packing fraction, and then applied it to calculate surface tension for liquid transition metals of the  $3d$ ,  $4d$  and  $5d$  series.

The many body potentials obtained by using embedded atom method (EAM) proposed independently by Daw, Baskes, [30,31] and Finnis and

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**Fig. 1.** Represents effective interionic interaction obtained from (a) BS pseudopotential and (b) many body EAM potentials. Solid, dashed, and dotted curves represent liquids Fe, Ag, and Pt, respectively.

Sinclair [32] have shown a good success in describing different properties of transition metals both in solid [30,33] and liquid phases [34–37]. The EAM version proposed by Bhuiyan et al. [38] has proved to be successful in describing the structure and thermodynamics of all liquid transition metals of the 3d, 4d, and 5d series and also for some rare earth metals [39]. Most importantly, Bhuiyan et al.'s version of EAM successfully predicted the liquid structure of Ti which has now been confirmed by levitation technique experiment [40]. On the other hand, Bretonnet and Silbert (BS) pseudopotential model [41] has proved to be useful for liquid 3d transition metals. The advantage of this model potential is that it can incorporate both *sp* and *d* band contributions within the framework of pseudopotential theory. In the present study, we have also chosen the Bretonnet–Silbert model as a serious test to see whether it works or not in describing surface tension of liquid transition metals.

This paper is organized in the following way. In Section 2 we briefly discuss both BS pseudopotential and, EAM potential. The liquid state theory used in this calculation is the variational modified hypernetted chain (VMHNC) integral equation theory which we discuss very briefly in this section. Expression used for the surface tension for is also presented in Section 2. The calculated results are presented in Section 3. The presented results are discussed in Section 4 and finally the paper is concluded in Section 5.

## 2. Theories

Theories relevant to the present study of surface tension are briefly described below.

### 2.1. Surface tension

From the scaled-particle theory [20], Mayer [28] proposed the following relationship for the compressibility,  $\chi$  and surface tension,  $\gamma$

$$\chi\gamma = \sigma \left[ \frac{2-3\eta + \eta^3}{4(1+2\eta^2)} \right] \quad (1)$$

where  $\sigma$  is the effective HS diameter and  $\eta$  is the packing fraction. The applicability of this relation is then confirmed by the study of Egelstaff et al. [42] for 30 liquids including liquid metals. Carnahan and Stirling [43] proposed the compressibility equation for HS fluid as

$$\chi = \frac{(1-\eta)^4}{nk_B T \{2\eta(4-\eta) + (1-\eta)^4\}} \quad (2)$$

where  $n$  is the ionic number density,  $k_B$  is the Boltzman constant and  $T$  is the temperature. Substitution of Eq. (2) into Eq. (1) yields

$$\gamma = \frac{\sigma nk_B T \{2\eta(4-\eta) + (1-\eta)^4\} (2-3\eta + \eta^3)}{4(1+2\eta^2)}. \quad (3)$$

Eq. (3) depends on  $\eta$  and  $\sigma$  which are also connected by the relation  $\eta = \frac{\pi\sigma^3 n}{6}$  [44].

### 2.2. Bretonnet and Silbert potential

Bretonnet and Silbert (BS) have proposed a model potential [41] for liquid transition metals. This model potential is constructed by the superposition of the *sp* and *d* band contributions,

$$w(r) = \begin{cases} \sum_{m=1}^2 B_m \exp\left(-\frac{r}{ma}\right) & \text{for } r < R_c \\ -\frac{Z_s e^2}{r} & \text{for } r > R_c \end{cases} \quad (4)$$

where  $a$ ,  $R_c$  and  $Z_s$  are the softness parameter, core radius and effective *s*-electron occupancy number, respectively. The unscreened form factor can be written as

$$w_0(q) = 4\pi m a^3 \left[ \frac{B_1 J_1}{(1+a^2 q^2)^2} + \frac{8B_2 J_2}{(1+4a^2 q^2)^2} \right] - \frac{4\pi m Z_s e^2 \cos(qR_c)}{q^2} \quad (5)$$

where the expressions for  $B_m$  and  $J_m$  are given in [41]. Now the effective interionic interaction is

$$v(r) = \frac{Z_s^2 e^2}{r} \left( 1 - \frac{2}{\pi} \int F_N(q) \frac{\sin(qr)}{q} dq \right) \quad (6)$$

where  $F_N(q)$  is the normalized energy wave number characteristic

$$F_N(q) = \left( \frac{q^2}{4\pi m Z_s e^2} \right)^2 w_0^2(q) \left[ 1 - \frac{1}{\epsilon(q)} \right] [1-G(q)]^{-1}. \quad (7)$$

The dielectric screening function  $\epsilon(q)$  is given by

$$\epsilon(q) = 1 - \left( \frac{4\pi e^2}{q^2} \right) \chi(q) [1-G(q)]. \quad (8)$$

Here  $\chi(q)$  is the Lindhard function and  $G(q)$  is the local-field correction as developed by Ichimaru and Utsumi [45].

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