

### Relationship between the Embedded-Atom Method and Tersoff Potentials

The expanding interest in modeling static structures and dynamic processes in condensed phases has led to the recent development of analytic many-body potential-energy expressions. The embedded-atom method (EAM) of Daw and Baskes<sup>1</sup> has proven to be an excellent formalism for describing interatomic forces in metals. Tersoff has introduced an apparently different expression<sup>2</sup> (based on earlier work by Abell<sup>3</sup>) that realistically describes bonding in covalently bonded solids such as silicon,<sup>2,4</sup> carbon,<sup>5,6</sup> and germanium.<sup>7</sup> This expression has also been used to describe bonding interactions in the gas-phase exchange reactions  $H+H_2$  and  $O+O_2$ .<sup>6</sup> Although initial efforts have been made toward using the EAM for silicon,<sup>8</sup> the two potential-energy expressions are generally used for different types of systems. In this Comment we show that for a reasonable choice of functional forms and parameters, the two expressions are identical.

Both the EAM and Tersoff functions express the binding energy as a sum over atomic sites, with the energy at each site being written as a pair sum plus a many-body function:

$$E_b = \sum_i E_i, \quad E_i = \frac{1}{2} \sum_{j(\neq i)} V_i^{\text{pair}}(r_{ij}) + V_i^{\text{mb}}, \quad (1)$$

where  $r_{ij}$  is the distance between atom  $i$  and atom  $j$ .

In the Tersoff expression the many-body term is

$$V_i^{\text{mb}} = -\frac{1}{2} \sum_{j(\neq i)} B b_{ij} e^{-\lambda_2 r_{ij}}. \quad (2)$$

Several functional forms have been proposed for  $b_{ij}$ . Tersoff has used

$$b_{ij} = \left[ 1 + \left( \sum_{k(\neq i,j)} G(\theta_{ijk}) e^{\lambda_3(r_{ij}-r_{ik})^3} \right)^n \right]^{-1/2n} \quad (3)$$

for his most recent silicon potentials,<sup>2(b),4</sup> and for his carbon<sup>5</sup> and germanium<sup>7</sup> potentials. The quantities  $n$  and  $\lambda_3$  in Eq. (3) are parameters, and an angular dependence enters through the function  $G(\theta)$ . A similar function of the form

$$b_{ij} = \left[ 1 + \sum_{k(\neq i,j)} G(\theta_{ijk}) e^{\lambda_3(r_{ij}-r_{ik})} \right]^{-\eta} \quad (4)$$

has been used for  $H_3$  and  $O_3$ .<sup>6</sup> Several other related forms have also been proposed,<sup>2,9,10</sup> including one without an explicit angular dependence.<sup>2(b)</sup>

In the EAM formalism the many-body term is

$$V_i^{\text{mb}} = -F \left( \sum_{j(\neq i)} \rho(r_{ij}) \right), \quad (5)$$

with  $F$  an embedding function and  $\rho(r_{ij})$  is the electron density at site  $i$  that is contributed by atom  $j$ . With the exception of the recent silicon potential<sup>8</sup> the atomic electron densities are assumed to be spherically symmetric.

Assuming an exponential form for the atomic electron density<sup>11</sup> and using the Finnis-Sinclair analytic expression for the embedding function,<sup>12,13</sup> Eq. (5) can be writ-

ten as

$$V_i^{\text{mb}} = -A \left( \sum_{j(\neq i)} e^{-ar_{ij}} \right)^{1/2}. \quad (6)$$

Equation (6) can be rewritten in the form of Eqs. (2) and (4) by the following algebra steps:

$$V_i^{\text{mb}} = -A \left\{ \sum_{j(\neq i)} e^{-ar_{ij}} \right\} \left[ \sum_{k(\neq i)} e^{-ar_{ik}} \right]^{-1/2} \quad (7a)$$

$$= -A \sum_{j(\neq i)} \left\{ e^{-ar_{ij}} \left[ \sum_{k(\neq i)} e^{-ar_{ik}} \right]^{-1/2} \right\} \quad (7b)$$

$$= -A \sum_{j(\neq i)} \left\{ e^{-ar_{ij}} \left[ e^{-ar_{ij}} + \sum_{k(\neq i,j)} e^{-ar_{ik}} \right]^{-1/2} \right\} \quad (7c)$$

$$= -\sum_{j(\neq i)} A e^{-ar_{ij}/2} \left[ 1 + \sum_{k(\neq i,j)} e^{a(r_{ij}-r_{ik})} \right]^{-1/2}. \quad (7d)$$

If  $B=2A$ ,  $\lambda_3=a=2\lambda_2$ ,  $\eta=\frac{1}{2}$ , and  $G(\theta)$  is taken as 1 [see Eq. (7) of Ref. 2(b)], then Eq. (7d) is identical to Eqs. (2) and (4). Also, in Abell's original paper<sup>3</sup> it was shown that the function  $b_{ij}$  can be identified as an effective Pauling bond order.<sup>14</sup> The relationship pointed out above then establishes a link between the Pauling bond order and the EAM formalism.

Of course the choices made above for the analytic functions do not reflect all of the forms used in the EAM and Tersoff potentials, but they do make the relationship between the two formalisms transparent. The main difference is the way in which angular interactions are incorporated.

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<sup>13</sup>Johnson has demonstrated that this choice of embedding function is essentially equivalent to other choices, differing only in a linear term in the sum of the electron densities (see Ref. 11).

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