



## Interatomic potentials for atomic scale modeling of metal–matrix ceramic particle reinforced nanocomposites

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### ABSTRACT

Functionally graded particle reinforced metal–matrix nanocomposite materials show significant promise for use in protective structures due to their high strengths, stiffness, failure resistance, and the ability to mitigate damage during ballistic impact. Further improvement of the performance of these materials requires fine-tuning of the nanostructure which, in turn, necessitates a clear fundamental understanding of the deformation and failure mechanisms under conditions of dynamic loading. While the molecular dynamics simulation technique is an excellent tool for investigation of the mechanisms of plastic deformation and failure of the particle reinforced metal–matrix nanocomposites at the atomic scale, the predictive power of the technique relies on an accurate description of the interatomic interactions. This paper provides a brief review of a recently developed class of interatomic potentials capable of the computationally efficient description of multi-component systems composed of metals, Si, Ge, and C. The potentials are based on reformulation of the Embedded Atom Method (EAM) potential for metals and two empirical potentials commonly used for covalently bonded materials, Stillinger–Weber (SW) and Tersoff, in a compatible functional form. The description of the angular dependence of interatomic interactions in the covalent materials is incorporated into the framework of the EAM potential and, therefore, the new class of potentials is dubbed Angular-dependent EAM (A-EAM) potentials. The A-EAM potentials retain all the properties of the pure components as predicted by the original SW, Tersoff, and EAM potentials, thus eliminating the need for extensive testing and limiting the scope of the potential parameterization to only the cross-interaction between the components. The performance of the A-EAM potentials is illustrated for the Au–Si system, with good agreement with experimental data obtained for the enthalpy of mixing in the Au–Si liquid alloy and the Au–Si phase diagram. The A-EAM potentials are suitable for large-scale atomistic simulations of metal–Si/Ge/C/SiC systems, such as the ones required for investigation of the dynamic response of nanocomposite materials to a ballistic/blast impact.

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### 1. Introduction

One of the long-standing problems in materials research has been the development and improvement of materials capable of withstanding ballistic/blast impact. These materials have often been referred to as blast and penetration resistant materials (BPRMs). Better materials lead to better resistance and, in turn, greater survivability. In addition to overall structural stiffness and strength, BPRMs require the ability to mitigate damage and provide ways to dissipate impact/blast energy. Metals have proven to be cost effective, high performing materials for protective structures, particularly the ones with high impact strengths. Another parameter, important to penetration resistance, is ductility. An

emerging class of materials for protective structures is functionally graded particle reinforced metal–matrix nanocomposites (MMnC) designed with compositional/structural gradients introduced through the variation of the concentration of the reinforcing ceramic particles (SiC, Al<sub>2</sub>O<sub>3</sub>, etc.) in the matrix [1,2]. Apart from their high strength, stiffness, and wear resistance, these nanocomposites have the ability to mitigate damage due to the spatial optimization of their properties. The trade-offs between the strength and ductility, observed in traditional metallic material systems, may not be applicable in these nanocomposites, leaving open the possibility of unprecedented performance improvements. The design and optimization of BPRM nanocomposite materials can be significantly accelerated by improvements in the understanding of the deformation and failure mechanisms under conditions of ballistic impact. Defense related loading conditions can result in impact velocities of a 1–2 km/s and peak strain rates of the order of

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$10^5$ – $10^6$  s $^{-1}$  [3]. The mechanisms responsible for plastic deformation and failure of MMnC are complex and are affected by multiple factors, such as the distribution and location/size of the reinforcing particles, grain size in the metal–matrix, characteristics of the interfaces between the particles and matrix grains, as well as the loading conditions [4].

While there has been significant progress in the understanding the mechanisms of the plastic deformation in MMnC under quasi-static loading conditions, the material behavior at high strain rates is still at a stage of the initial exploration. The lack of detailed information on the response of the nanocomposite materials to the fast dynamic loading is related to the small time scales involved and the heterogeneous nature of these materials, which make it difficult to identify and characterize the elementary processes responsible for plastic deformation and failure using experiments alone. The molecular dynamics (MD) simulation technique has a potential of providing the atomic level structural information on the deformation mechanisms at high strain rates [5] and may be instrumental in physical interpretation of experimental observations. MD simulations of plastic deformation are typically carried out at strain rates  $\geq 10^7$  s $^{-1}$ . While these strain rates are higher than conventional strain rates in ballistic impact experiments, the current state-of-art simulations boast up to 350 billion atoms of copper corresponding to 1.56  $\mu$ m size systems [6], as well as investigations of shock-induced phase transformations in multi-million atom samples [7]. With the increasing availability of computing resources, it should be possible to model deformation of systems comprising of many billions of atoms at realistic strain rates in the near future. Although the capabilities of MD method for investigations of mechanical behavior and properties of real materials are very promising, its ability to provide reliable quantitative information is, in a big part, defined by the availability of accurate and computationally efficient interatomic potentials.

Over the last several decades, a broad variety of empirical and semi-empirical potentials have been suggested in literature. For many of the potentials, however, the verification of their predictive power has been limited to relatively narrow domains of physical conditions, directly relevant to their applications in the initial studies. As a result, out of the vast number of potentials developed, only a relatively small fraction has been thoroughly tested and found to exhibit a combination of transferability, computational efficiency, and simplicity of implementation that ensures their broad use by many research groups. In particular, the Embedded Atom Method (EAM) [8–11] has provided the framework for a group of potentials that are used in the majority of current simulations of metals and metallic alloys. Popular potentials for covalently bonded systems include Stillinger–Weber (SW) potential [12,13] for Si and Ge, Tersoff potential [14,15] for Si and C, as well as Brenner potential [16,17] for hydrocarbon systems. The extension of the empirical potentials to alloys consisting of components with the same type of interatomic bonding (and described by the same type of interatomic potential) is relatively straightforward, with several alloy models (schemes for the description of cross-interactions between the components) developed for metals [11,18–21] and covalent systems [22,23]. The design of interatomic potentials capable of an adequate description of multi-component systems with mixed types of atomic bonding, however, is a more challenging task that has to be addressed to enable atomic scale modeling of a range of practically important systems. Computationally efficient and accurate description of systems with mixed metallic–covalent bonding, in particular, is highly desirable for investigation of the mechanical properties of metal–matrix nanocomposites reinforced by ceramic nanoparticles.

The Modified Embedded Atom Method (MEAM) potential [24] by Baskes includes parameterization for many cubic metals, as well as Si, Ge, C, H, N, and O. The potential, therefore, can be adopted for

modeling of systems with mixed type of bonding, such as Mo–Si [25], Au–Si [26], and Au–Si–O [27]. A many-body angular screening function, used as a cutoff mechanism in MEAM, however, makes this potential to be computationally expensive. Moreover, the properties of both pure components and mixtures predicted by the MEAM potential have to be verified for each system of interest. An adjustment of the parameters of the MEAM potential, therefore, is often required in order to achieve an adequate description of the pure components [28]. Several potentials have been suggested for modeling of complex systems such as SiO $_2$  [29,30], SiC [31], and Alumina [32], with the charge transfer between the components explicitly incorporated into the models. The applicability of these potentials to study the pure elements and/or their interfaces with metallic systems has not been addressed.

An attractive alternative to the design of new alloy potentials with original functional forms can be provided by combination of well-established and thoroughly tested potentials developed for pure components within a unified approach. Despite the differences between the functional forms and underlying physical arguments used in the description of interatomic bonding in metallic and covalent systems, there has been a number of works suggesting the feasibility of the unified approach. In particular, a description of Pt–C system with an analytical potential that, for pure components, reduces to the bond-order Brenner potential for C and an EAM-like potential for Pt has been discussed by Albe et al. [33]. The connections between the EAM formalism and the bond-order scheme of the Tersoff potential have been discussed by Brenner [34], whereas the relationship between the SW and MEAM potentials has been discussed by Thijssse [35], who shows that the two potentials can be reformulated into compatible functional forms.

In this paper, we discuss the basic ideas and the functional form of a newly developed class of Angular-dependent EAM (A-EAM) potentials [36,37]. The A-EAM potentials incorporate a description of the angular dependence of interatomic interactions into the general framework of the EAM potential, making them compatible with the SW and Tersoff potentials. The A-EAM potentials retain all the properties of the pure components as predicted by the original SW, Tersoff, and EAM potentials, thus eliminating the need for extensive testing and limiting the extent of the parameterization needed. The reformulation of the EAM, SW, and Tersoff potentials leading to the development of the unified A-EAM potentials is described in Section 2. The ability of the A-EAM potentials to provide an adequate description of binary systems with mixed type of bonding is illustrated in Section 3, where some of the thermodynamic properties of the Au–Si alloy represented by an A-EAM potential are discussed.

## 2. The Angular-dependent Embedded Atom Method

A unified alloy potentials based on a reformulation of the EAM, SW, and Tersoff potentials in a compatible functional form are discussed in this section. A reformulation of the conventional EAM potential into a general A-EAM form that includes three-body terms in the expression for the total electron density function is presented first, followed by a description of two approaches developed for incorporation of the angular dependence compatible with either SW or Tersoff potentials.

### 2.1. EAM potential with three-body terms in the electron density function

In the EAM potentials, the energy of an atom is expressed as

$$E_i = \frac{1}{2} \sum_{j \neq i} \phi_{ij}(r_{ij}) + F_i(\rho_i), \quad (1)$$

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