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# ZMODYFIKOWANY POTENCJAŁ RGL DLA METALI ŚCIENNIE CENTROWANYCH

# MODIFIED RGL POTENTIAL FOR FCC METALS

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***ABSTRACT***

The main goal of this paper is to examine a modification of the EAM (embedded atom model) type molecular potential by Rosato-Guillope-Legrand (RGL) to improve description of mechanical properties of FCC structures ) [2]. The proposed potential correctly reproduces the crystal behavior not only in the range of small strains but also at finite deformations. In addition to correctly predicting the cohesive energy, elastic and lattice constants, the stacking fault energy also remains in good agreement with experiment.

A certain group of the EAM potentials is based on the Second Moment Approximation of the Tight-Binding Hamiltonian (TB-SMA) [2]. The approach is a result of the observation that a large set of properties of transition metals can be derived purely from the density of states of the outermost *d* electrons. From experiments it is known that the cohesive energy of metals is roughly proportional to the width of the density of states described by the square root of the second moment: $(\mu_2)^{1/2}$. This is the basis of the second-moment approximation.

According to the original RGL potential, the crystal energy per atom is a sum of the repulsive Born-Mayer term, and attractive square root operation - giving the embedding function *F*:

$$E_{at} = \sum_i A e^{-p\left(\frac{r_i}{r_o}-1\right)} - \left(\sum_i \zeta^2 e^{-2q\left(\frac{r_i}{r_o}-1\right)}\right)^{\frac{1}{2}}, \qquad (1)$$

Here $r_0$ is the equilibrium distance between the nearest atoms and $A$, $p$, $\zeta$ and $q$ are fitted parameters. Although the model has a simple functional form, it can be used to well describe the cohesive energy, elastic and lattice constants of a wide range of FCC- and HCP-metals (mainly transition).

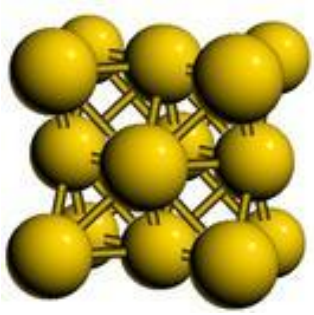

Figure 1: The Face-Centered Cubic (A1) Lattice.

The weakness of the original RGL potential is generally an underestimation of the stacking fault energy [1] and lower accuracy for non-transition metals. We modify the attractive part of the potential in Eq. (1) and utilizing a symmetry-based approach [1] and molecular statics calculations [3] we fit the parameters of the modified potential for copper and aluminium to reduce the weaknesses of the original one.

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