Supporting Information for:

The Impact of Short-range Forces on Defect Production from High-energy Collisions

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S1. Equation of state and dimer energy in the EAM formalism

The energy of a single element crystal lattice per atom can be written within the EAM formalism as:

$$E(a) = \frac{1}{2}\sum_{i \in N_n} N_i \varphi(\alpha_i a_o) + F(\bar{\rho}) \ , \qquad \text{(S1)}$$

where

$$\bar{\rho} = \sum_{i \in N_n} N_i \rho(\alpha_i a_o)$$

is the local density at a site i and sum goes over all the neighboring shells. N_i is the number of atoms in the i-th shell and the term $\alpha_i a_o$ is the distance between a given site and atoms in the specified shell. The symbol a_o is the lattice parameter. The number of atoms and the distances associated with the first six neighbor shells are listed in Table S1.

Table S1: Number of atoms and distances from origin for first six nearest neighbor shells for an fcc lattice

Shell	1	2	3	4	5	6
N_i	12	6	24	12	24	8
α_i	$\sqrt{0.5}$	1.0	$\sqrt{1.5}$	$\sqrt{2.0}$	$\sqrt{2.5}$	$\sqrt{3.0}$

The error introduced by using a finite number of neighbor shells can be reduced by rewriting Eq. (S1) in terms of differences with respect to the equilibrium energy, E_0:

$$E(a) = E_0 + \frac{1}{2}\sum_{i \in N_n} N_i\big(\varphi(\alpha_i a) - \varphi(\alpha_i a_0)\big) + F(\bar{\rho}_0 + \Delta\bar{\rho}) - F(\bar{\rho}_0) \qquad \text{(S2)}$$

$$\Delta\bar{\rho} = \sum_{i \in N_n} N_i\big(\rho(\alpha_i a) - \rho(\alpha_i a_0)\big) \quad \text{(S3)}$$

Similar to the case for the analytical EOS, a formula can be written for the dimer energy in the crystal lattice. The formula has the following form:

$$E(r) = E_0 + \frac{1}{2}\sum_{i \in N_n} N_i\big(\varphi(r_i(r)) - \varphi(r_i(r_0)\big) + F(\bar{\rho}_0 + \Delta\bar{\rho}) - F(\bar{\rho}_0) \qquad \text{(S4)}$$

$$\Delta\bar{\rho} = \sum_{i \in N_n} N_i\big(\rho(r_i(r)) - \rho(r_i(r_0))\big) \qquad \text{(S5)}$$

The term N_i is related to the number of atoms contributing, which for the case $i = 1$ involves only the nearest neighbor. The distance function $r_i(r)$ is shown in Table S2 for different site contributions, where the term r_0 is the equilibrium separation between nearest neighbor atoms.

Table S2: Terms contributing to sum in Eqns. (S4) and (S5)					
Contribution	1	2	3	4	5
N_i	1	4	2	4	1
$r_i(r)$	r	$\sqrt{r^2 - rr_0 - r_0^2}$	$\sqrt{r_0^2+(r_0 - r)^2}$	$\sqrt{3r_0^2 - 3rr_0 + r^2}$	$2r_0 - r$

S2. LAMMPS overlay method for joining ZBL to equilibrium potentials

The LAMMPS hybrid/overlay method can be used to superimpose two interatomic potentials such as joining the ZBL to an EAM potential at short atomic separation distances[S1]. The general form is:

$$E(\mathbf{r}) = E_{EAM}(\mathbf{r}) + E_{ZBL+S}(\boldsymbol{r}). \qquad \text{(S6)}$$

The ZBL implementation of LAMMPS requires that the user provide the atomic number of the interacting atoms, as well as an inner cutoff (r_1) and outer cutoff (r_c) radius. The outer cutoff radius is the global cutoff distance for the ZBL interaction, while the inner cutoff radius is the distance where a "switching" function, *S(r)*, is used to smoothly join the ZBL to the equilibrium potential:

$S(r) = C \qquad r < r_1$	
$S(r) = \frac{A}{3}(r - r_1)^3 + \frac{B}{4}(r - r_1)^4 + C \qquad r_1 < r < r_c$	
$A = (-3E'_{ZBL}(r_c) + (r_c - r_1)E''_{ZBL}(r_c))/(r_c - r_1)^2$	(S7)
$B = (2E'_{ZBL}(r_c) + (r_c - r_1)E''_{ZBL}(r_c))/(r_c - r_1)^3$	
$C = -E_{ZBL}(r_c) + \frac{1}{2}(r_c - r_1)E'_{ZBL}(r_c) - \frac{1}{12}(r_c - r_1)^2E''_{ZBL}(r_c)$	

This switching function is added to the ZBL interaction:

$$E_{ZBL+S}(r) = E_{ZBL} + S(r) \qquad r < r_c. \qquad \text{(S8)}$$

References

S1. The LAMMPS overlay method is described in the on-line manual at: http://lammps.sandia.gov/doc/pair_hybrid.html, http://lammps.sandia.gov/doc/pair_zbl.html, http://lammps.sandia.gov/doc/pair_gromacs.html, (Accessed Dec. 15, 2015).