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https://arxiv.org/pdf/1904.00360

Deep learning inter-atomic potential model for accurate irradiation damage simulations

Ziegler-Biersack-Littmark-modified deep learning scheme

System energy:

$$E^{\text{ZBL-DP}} = \sum_i E_i^{\text{ZBL-DP}}$$

The atomic contribution of atom i is fully determined by the coordinates of atom i and its near neighbors:

$$E_i^{\text{ZBL-DP}} = E_{s(i)}^{\text{ZBL-DP}}\left(\boldsymbol{R}_i, \{\boldsymbol{R}_j | j \in \mathcal{N}_{R_c}(i)\}\right)$$

Ziegler-Biersack-Littmark-modified deep learning scheme

The atom contribution of DP-ZBL is the interpolation of the ZBL screened nuclear repulsion potential E^{ZBL} i and the standard deep potential E^{DP}

$$E_i^{\text{ZBL-DP}} = w_i E_i^{\text{ZBL}} + (1 - w_i) E_i^{\text{DP}}$$

$$w_i = \begin{cases} 1 & \sigma_i < R_a, \\ -6u_i^5 + 15u_i^4 - 10u_i^3 + 1 & R_a \le \sigma_i < R_b \\ 0 & \sigma_i \ge R_b, \end{cases}$$

Ziegler-Biersack-Littmark-modified deep learning scheme

$$u_i = \frac{\sigma_i - R_a}{R_b - R_a}$$

Smooth-minimal distance of atom i's near neighbors:

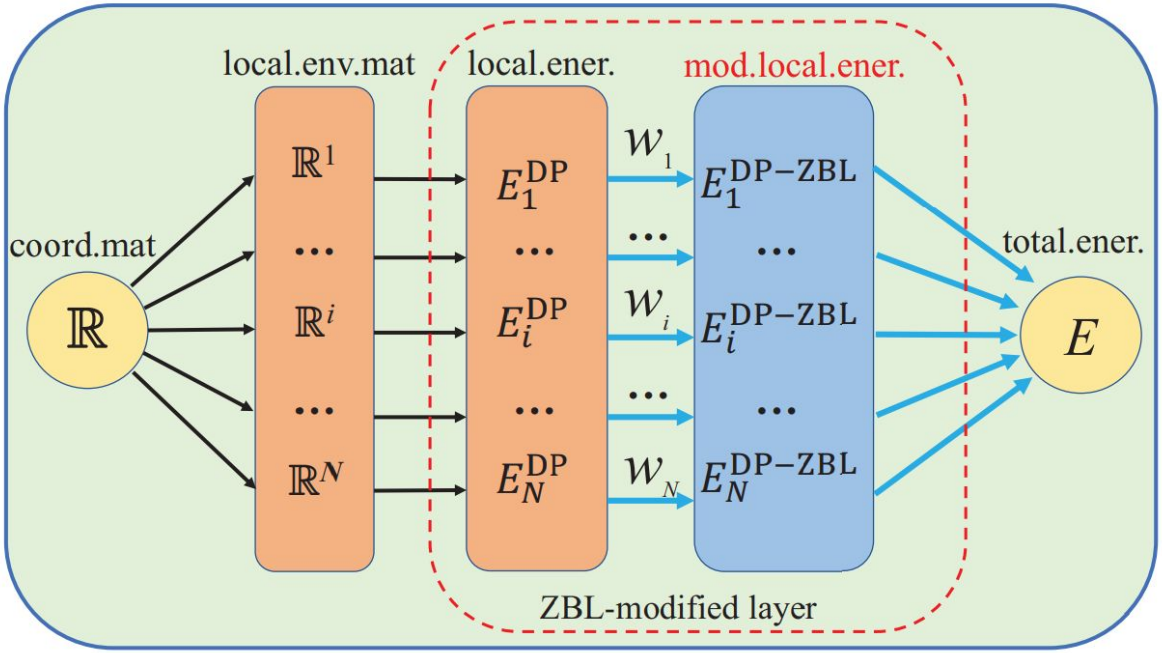
$$\sigma_i = \frac{\sum_{j \in \mathcal{N}_{R_c}(i)} R_{ij} e^{-R_{ij}/\alpha}}{\sum_{j \in \mathcal{N}_{R_c}(i)} e^{-R_{ij}/\alpha}},$$

Equilibrium properties of Al

Al[a]	EXP.	DFT	DP-ZBL	DP[24]	MEAM-ZBL	EAM-ZBL[b]
E_{am} [eV/atom]	-3.49[25]	-3.75	-3.74	-3.65	-3.36	-3.39
a_0 [Å]	4.04[26]	4.04	4.04	4.04	4.05	4.01
E_{vf} [eV]	0.66[27,28]	0.67[29]	0.73	0.79	0.67	1.14
$E_{if}(oh)$ [eV]	-	2.91[29]	2.57	2.45	3.12	-
$E_{if}(th)$[eV]	-	3.23[29]	3.23	3.12	3.83	-
C_{11} [GPa]	114.3[30]	111.2	112.8	120.9	113.5	106.9
C_{12} [GPa]	61.9[30]	61.4	57.6	59.6	61.6	81.5
C_{44} [GPa]	31.6[30]	36.8	41.2	40.4	45.4	44.2
B_V [GPa]	79.4[30]	78.0	76.0	80.1	78.9	90.0
G_V [GPa]	29.4[30]	32.1	35.8	36.5	37.6	31.6
$\gamma_{sf}[J/m^2]$	0.11-0.21[31–34]	0.142[35]	0.070	0.132	0.184	-
$\gamma_{tsf}[J/m^2]$	-	0.135[35]	0.075	0.130	0.184	-
T_m [K]	935[36]	950(±50)[37]	885	918	950	1050
ΔH_f [KJ/mol]	10.7(± 0.2)[38]	-	9.3	10.2	11.5	8.8
$D[10^{-9}m^2/s]$	7.2-7.9[39]	-	6.8	7.1	4.9	6.8

Atomization energy Eam, equilibrium lattice constant a0, vacancy formation energy Evf, interstitial formation energy Eif for octahedral interstitial (oh) and tetrahedral interstitial (th), independent elastic constant C11, C12, and C44, Bulk modulus BV (Voigt), shear modulus GV (Voigt),stacking fault energy γsf, twin stacking fault energy γtsf, melt point Tm, enthalpy of fusion ΔHf and diffusion coefficient D at T = 1000 K.

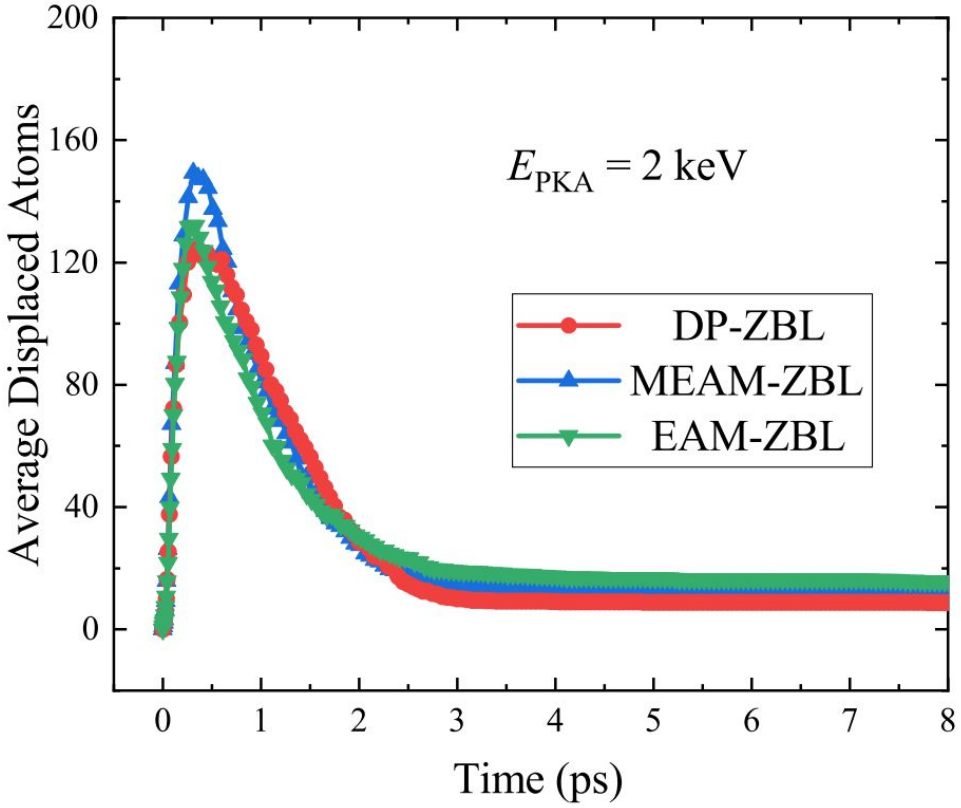
Schematic plot of the DP-ZBL model



Coordinate matrix R to the potential energy E, R is firstly transformed to local environment matrices. Then each R^i is mapped and ZBL-modified layer is added

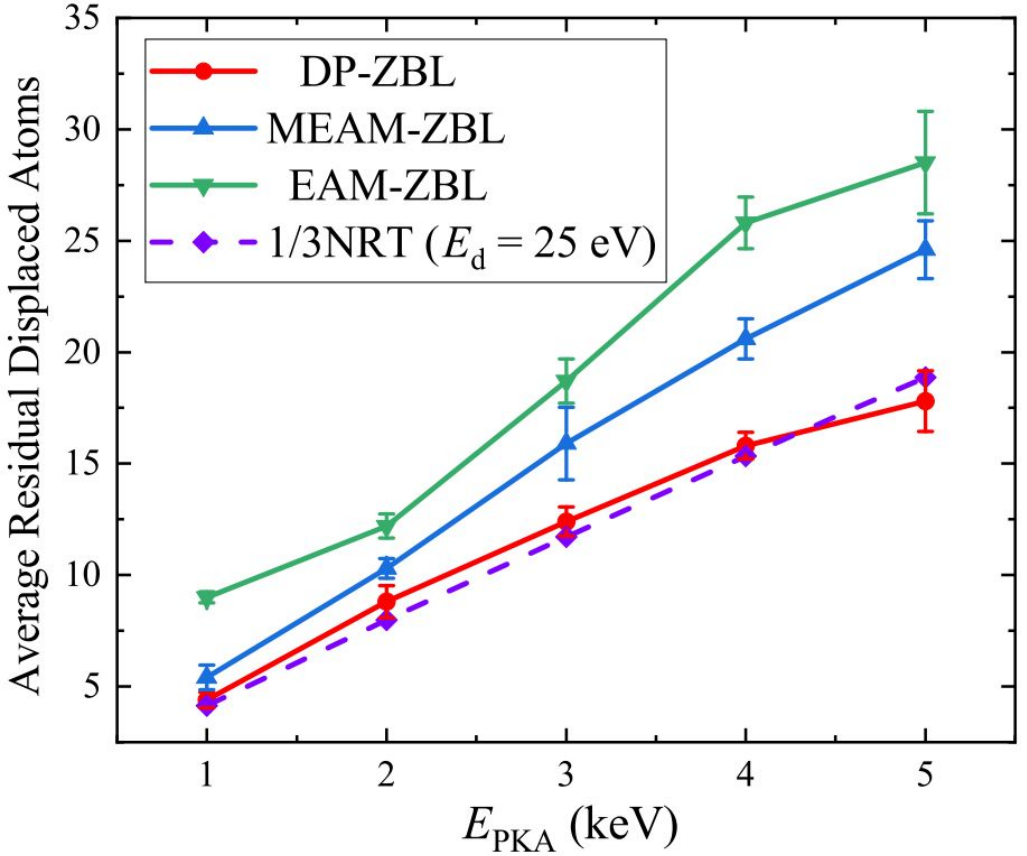
Average displaced atoms

The number of average displaced atoms Nd during the evolution of the collision cascade caused by a 2 keV PKA. Each point is the average of 10 independent 2 keV cascade simulations.



Point defects after 50 ps relaxation

The residual point defects after 50 ps relaxation and the corresponding 1/3 NRT model results. Each point is the average of 10 independent cascade simulations, and the errors are given in the standard error of the mean



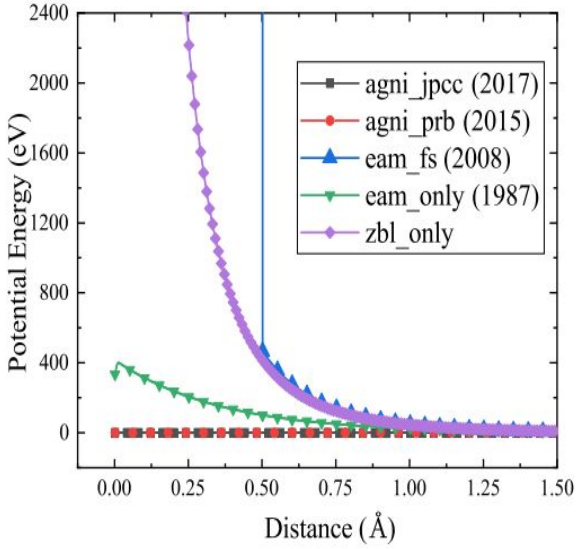
Conclusions

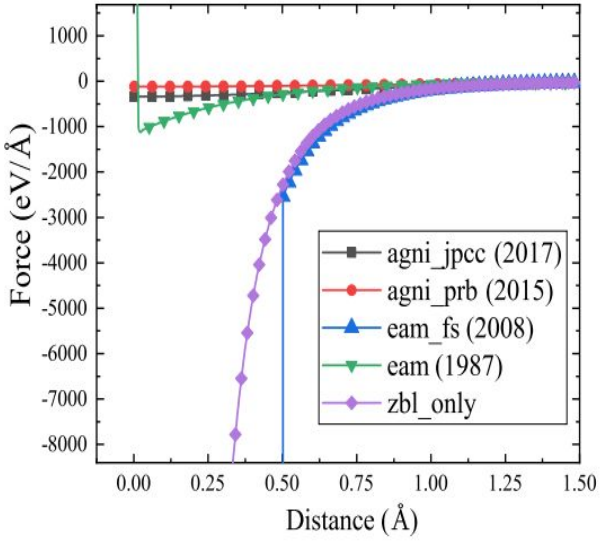
The average displacement threshold energy (Ed) of fcc Al

fcc Al	Recommended[66]	DP-ZBL	MEAM-ZBL	EAM-ZBL
E_d (eV)	25.0	26.54	22.67	16.73

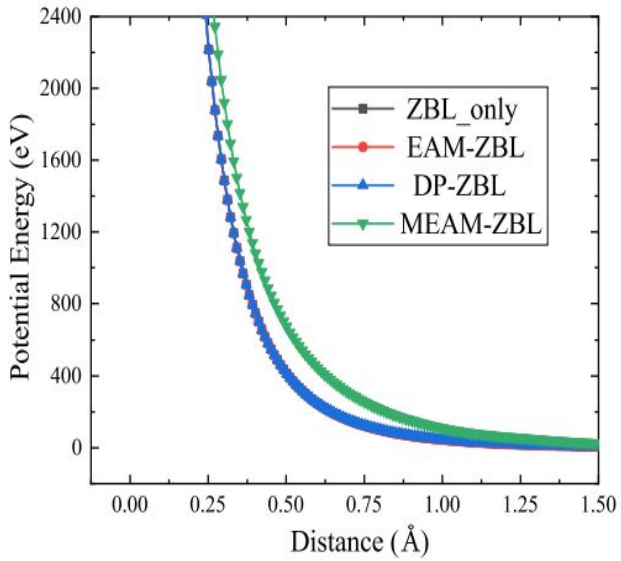
- Proposed DP-ZBL scheme by smoothly interpolating the accurate repulsive pair potential (ZBL) into the DP model
- Not only give accurate results regarding the material properties near equilibrium states but also sufficient to describe the atomic collision cascades during the irradiation damage processes
- Minimize the impact of subjective factors on potentials during their establishments
- May be used in the irradiation effect studies of new advanced materials, such as high entropy alloys, layered transition metal ternary nitrides and carbides, and 2D materials, for whom suitable classical potentials are still lacking

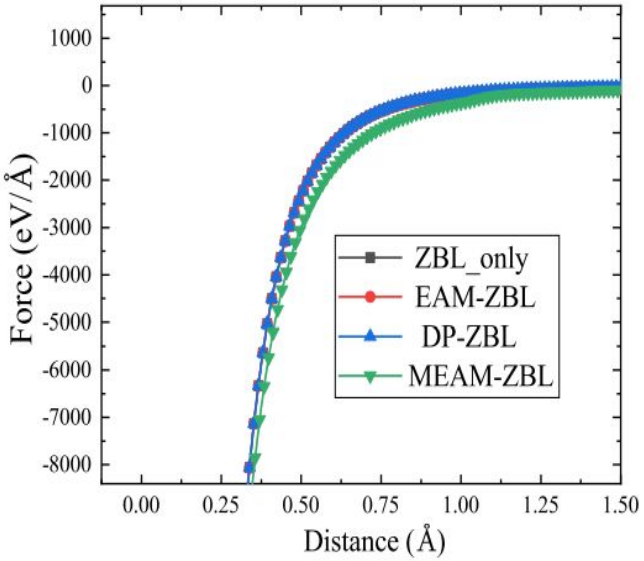
The pair potential (a) and force (b) calculated using two classical potentials (eam and eam.fs) and two machine learning potentials (agni_jpcc and agni_prb). Compared the ZBL repulsive pair potential, all the four potentials cannot give an accurate description about the interatomic interactions below 1 Å.



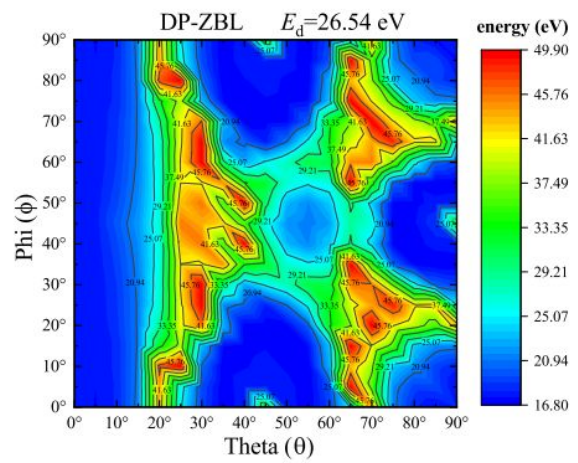


The pair potential (a) and force (b) calculated using the DP-ZBL, EAM-ZBL and one state-of-art classical potentials MEAM-ZBL. As all these potentials are smoothly transformed into the ZBL repulsive potential at short distance, they are sufficient to describe the interatomic interactions during the cascade simulations.

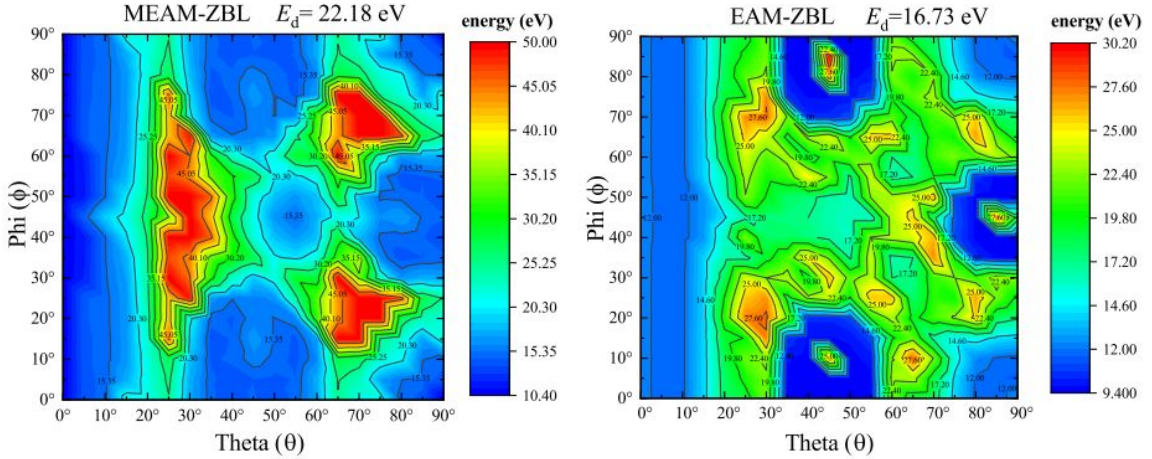




The corresponding Ed(θ,φ) calculated using the (a) DP-ZBL, (b) MEAM-ZBL, and (c) MEAM-ZBL potentials. All the three potentials show similar dependence of Ed on the PKA initial direction (θ,φ)



(a)



(b) (c)

The evolution of average displaced atoms number (Nd) during the cascades events induced by 1 keV(a), 3 keV (b), 4 keV (c) and 5 keV (d) PKAs. Each point is the average of 10 independent simulations.