An Impasse in MD simulations of Primary Damage: Which Interatomic Potential yields the correct defect morphology

Manoj Kumar Warrier[a,b] & Utkarsh Bhradwaj[a]

[a] Computational Analysis Division, Bhabha Atomic Research Center, Visakhapatnam, India

[b] Homi Bhabha National Institute, Anushaktinagar, TROMBAY, Mumbai, India

Aim Compare the primary damage resulting from collision cascades in W from three widely used EAM based interatomic potentials (JW [1], MS [2] & DND-BN [3]) with two recently developed Machine Learning potentials (WSNAP [4], tabGAP [5]) with sufficient statistics

LAMMPS [6] **simulations of Collision Cascades** in W with JW, MS, DND-BN, WSNAP and tabGAP IAP

- 100 random directions at each energy
- NVE simulations with variable timestep using a Fixed outer boundary with T control in penultimate cells

S.No	PKA Energy (keV)	Simulation Size	No. of Atoms
1	5	$50 \times 50 \times 50$	250000
2	10	$75 \times 75 \times 75$	843750
3	20	$85 \times 85 \times 85$	1228250
4	50	$100 \times 100 \times 100$	2000000
5	75	$125 \times 125 \times 125$	3906250
6	100	$150 \times 150 \times 150$	6750000
7	150	$200 \times 200 \times 200$	16000000

IAP stiffening parameters

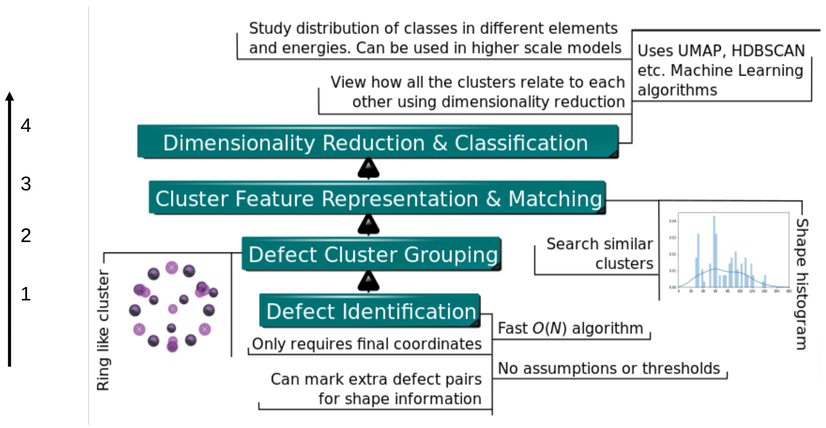
IAP	r1 (Å)	r2 (Å)	R (Å)	S	S/R ($Å^{-1}$)
JW	1.39	2.6	1.4	-150	-107
DND-BN	1.1	2.25	1.3	-230	-177
MS	1.3	2.0	1.45	-137	-95
WSNAP	ZBL	ZBL	1.4	-145	-104
tabGAP	SC	SC	1.27	-223	-176

Table comparing the material properties obtained using the five IAP with published DFT simulations and Experimental results (erors from the comparison are given in brackets – **large errors are highlighted**)

	Property	DFT	Expt.	JW	MS	DND-BN	WSNAP	tabGAP
Lattice Parameter →	a (Å)	3.18	3.17	3.17 (0.15)	3.16 (-0.16)	3.16 (0.0)	3.18 (-0.15)	3.18 (-0.16)
Coeficients of stiffness tensor & Elastic modulii	C11 (GPa)	521	522.0	475.33 (-8.77)	517.41 (-0.69)	544.18 (4.25)	538.99 (3.25)	564.87 (8.21)
	C12 (GPa)	195	204.0	195.29 (0.15)	7258.66 (**26.79**)	350.89 (**72.01**)	208.73 (2.32)	207.92 (1.92)
	C44 (GPa)	147	161.0	154.63 (-3.96)	186.11 (15.59)	242.37 (**50.54**)	152.92 (4.03)	152.15 (3.51)
	B (GPa)		310.0	288.64 (-6.89)	344.91 (9.5)	415.32 (**31.85**)	318.82 (1.21)	326.90 (3.78)
	S (GPa)		161.0	148.79 (-7.59)	163.42 (1.5)	184.08 (10.89)	157.80 (-1.99)	162.68 (1.04)
Poisson Ratio →	ν		0.28	0.29 (4.0)	0.33 (19.03)	0.39 (**40.01**)	0.28 (-0.3)	0.27 (-3.91)
Defect formation energies	VFE (eV)	3.36	3.80	3.65 (-3.95)	3.86 (1.64)	3.58 (5.91)	3.13 (-6.84)	3.31 (-1.43)
	SIA-Oct (eV)	12.27	10.5	10.26 (-2.24)	11.58 (-5.59)	11.53 (-6.06)	12.34 (0.57)	12.23 (-0.34)
	SIA-Tet (eV)	11.72	11.2	10.29 (-8.16)	10.88 (-2.9)	10.83 (-3.31)	11.82 (0.84)	12.50 (6.61)
	SIA-DB-100 (eV)	12.2	11.5	10.15 (-11.75)	11.87 (-2.7)	11.34 (-1.39)	11.60 (0.87)	12.43 (1.89)
	SIA-DB-110 (eV)	10.58	10.60	9.99 (-5.58)	9.78 (-7.59)	9.68 (-8.49)	10.39 (-1.78)	11.28 (6.38)
	SIA-DB-111 (eV)	10.29	10.30	9.55 (-7.17)	9.65 (-6.21)	9.37 (-8.98)	10.33 (0.26)	11.14 (8.17)
	DB 110-111 (eV)	0.3	0.30	0.44 (**-50.98**)	0.13 (**56.76**)	0.32 (-8.65)	0.06 (**77.81**)	0.13 (**53.69**)
Coefficient of thermal expansion →	$\alpha(K^{-1})$	4.9e-6	4.5e-6	8.74e-6 (**-78.32**)	5.19e-6 (-5.87)	-9.72e-7 (**119.83**)	7.14e-6 (**-45.72**)	6.79e-6 (**-38.59**)
Threshold Displacement Energies	TDE mean (eV)		90.0	133.79 (**48.65**)	96.79 (7.54)	100.57 (11.75)	111.79 (**24.21**)	109.85 (**22.06**)
	TDE max (eV)			249.0	199.70	163.00	220.70	187.70
	TDE min (eV)			54.3	43.00	42.30	45.70	38.30
	TDE 100 (eV)		42.0	54.30 (**-29.29**)	43.00 (-2.38)	42.30 (-0.71)	45.70 (-8.81)	38.30 (8.81)

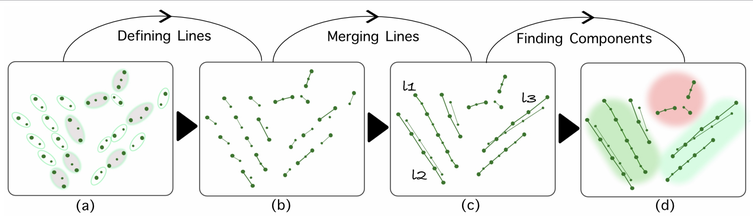
All IAP have mismatch with experiments / DFT. Whilst DND-BN looks good for defect formation studies, it will be bad for Swelling studies (thermal expansion and elastic constants). Thermal expansion is bad for all IAP except MS, which due to the large error in DB110-111 ends up giving more <110> defects than DND-BN. The DFT and Expt values are obtained from [4,7] and references therein.

Post Processing: Classifying defect clusters using ML



CSaransh: AI/ML based algorithm to classify defects
https://github.com/haptork/csaransh
[Computational Materials Science 172 (2020) 109364]

Post Processing: Obtaining morphology, internal morphology and orientation using Graph Data Structure



- Each line is the **node** of a graph
- **Edges** connecting the nodes are made using
- (i) angles between the lines
- (ii) distance between the lines
- **Dijkstra's algorithm** to find **connected homogeneous** regions

SAVI: Graph algorithm to obtain the internal morphology and orientation of defect clusters.
[Computational Materials Science 195 (2021) 110474
Mod. Sim. Mater. Science & Engg.,29 (2021) 065015]

Results: Here instead of figure captions (which are obvious), observations are noted as captions to guide the thought process

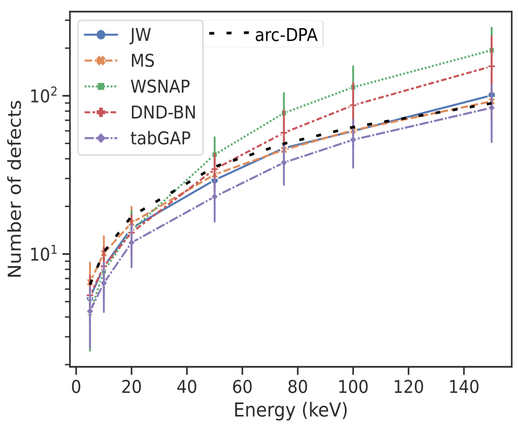


Fig.1: Good match with arc-DPA **Inverse correlation with number of Sub-cascades (Fig.6).**

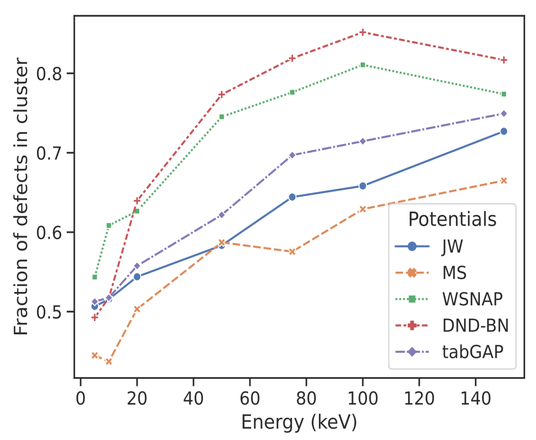


Fig.2: Clear heirarchy amongst IAP

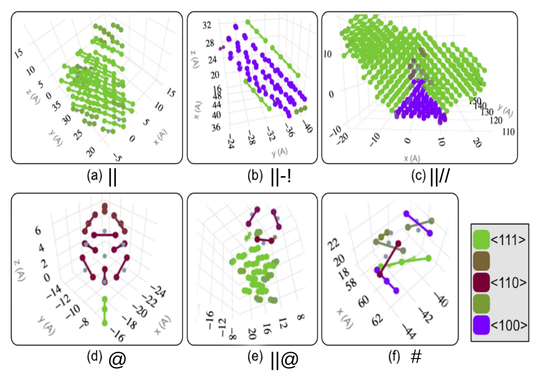


Fig.3: Cluster classes. Note ascii symbols of each cluster class. **Hexagonal rings have <110> defects**

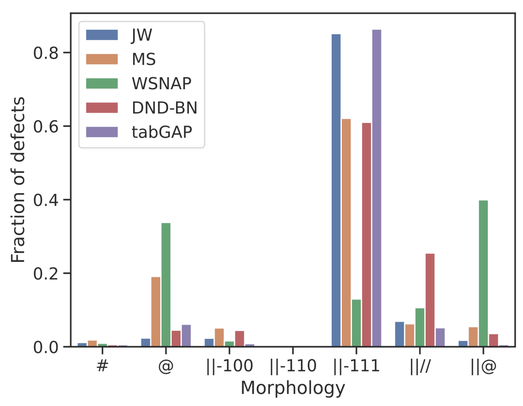


Fig.4: **Difference in formation energy between <110> and <111> components decide if rings are formed or not! D 110-111 decides @ formation** (see property table above.
The values for this parameter are WSNAP > MS=tabGAP >> DND-BN > JW which match the fraction of **"@"**!

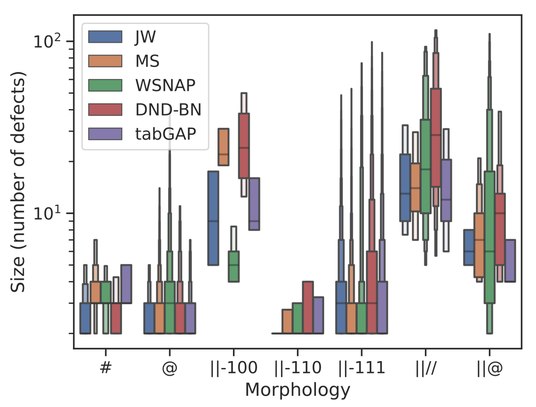


Fig.5: The "||-!" and "||//" clusters are The biggest. Some "||" can be large

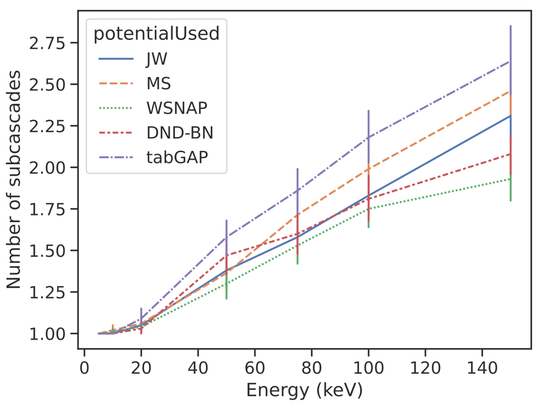


Fig.6: Number of sub-cascades show an inverse correlation with the number of defects. We use HDBScan algorithm to obtain the number of sub-cascades [Modelling and Simulations in Mater. Sci. & Engg. 32 (5) (2024) 055017]

Conclusions

- **Number of sub-cascades show an inverse correlation with the number of defects (Figs.1 & 6).**
- **Difference in formation energy between <110> and <111> components decide if rings are formed or not!** The values for this parameter are WSNAP > MS=tabGAP >> DND-BN > JW. The values for this parameter are WSNAP > MS=tabGAP >> DND-BN > JW which match the fraction of **"@" (fig.4 & 14th row big table above)**! All IAP which have been trained on liquid configurations have a low value for this parameter and form rings ("@").
- **All IAP have mismatch with experiments / DFT**. Whilst DND-BN looks good for defect formation studies, it will be bad for Swelling studies (thermal expansion and elastic constants). Thermal expansion is bad for all IAP except MS, which due to the large error in DB110-111 ends up giving more <110> defects than DND-BN.

References

1) N. Juslin, B. Wirth, Journal of Nuclear Materials 432 (1) (2013) 61 – 66
2) A. Sand, et al., Journal of Nuclear Materials 470 (2016) 119–127.
3) C. Björkas, et al., Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 267 (18) (2009) 3204 – 3208.
4) M. A. Wood, A. P. Thompson, (2017) arXiv:1702.07042.
5) J. Byggmästar, et al., Physical Review B 104 (10).
6) A. P. Thompson, et al., Comp. Phys. Comm. 271 (2022) 108171.
7) J. Byggmästar, et al., (2020) arxiv:2006.14365v2

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