Supplementary material

Formation of Interstitial Dislocation Loops by Irradiation in Alpha-Iron under Strain: A Molecular Dynamics Study

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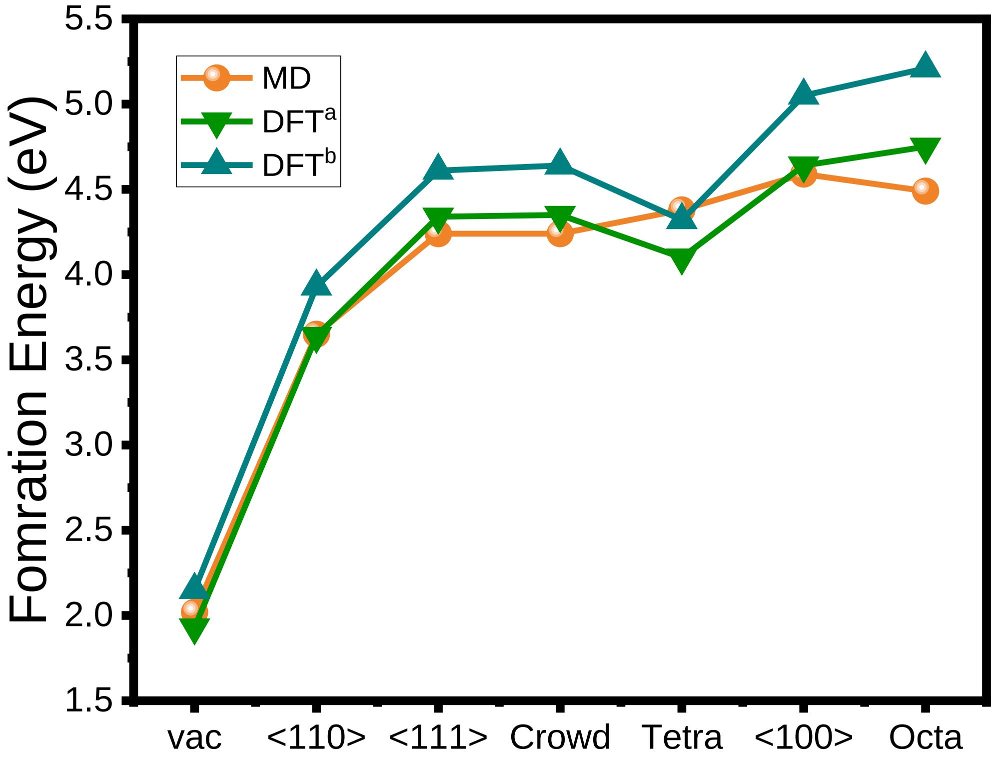


E_m^v (eV)	**0.67**[c]	**0.79**
E_m^{sia} (eV)	0.34[c]	0.25

Fig. S1 a comparative study for the interstitial formation energies of current molecular dynamic study (MD) study potential model with the density functional theory (DFT) calculations at free strain. The E_m^v and E_m^{sia} are the vacancy and self-interstitial (sia) migration energies.

[a] Reference [1]

[b] Reference [2]

[c] Reference [3]

Table S1. The comparison of the MD and DFT directional threshold displacement energy ($E_{d,i}$)

(i = <100> , <110> and <111>) and the average threshold displacement energy ($E_{d,avg}$) values referenced to the experiential results.

	E_d (100)	E_d(110)	E_d(111)	$E_{d,avg}$
MD	20	48.7	43	38.6
DFT_{psd}[a]	21	43	20	32
Experiment [b]	17	>30	20	
Experiment [b]	20	20	30	

[a] Reference [4]

[b] Reference [5]

[c] Reference [6]

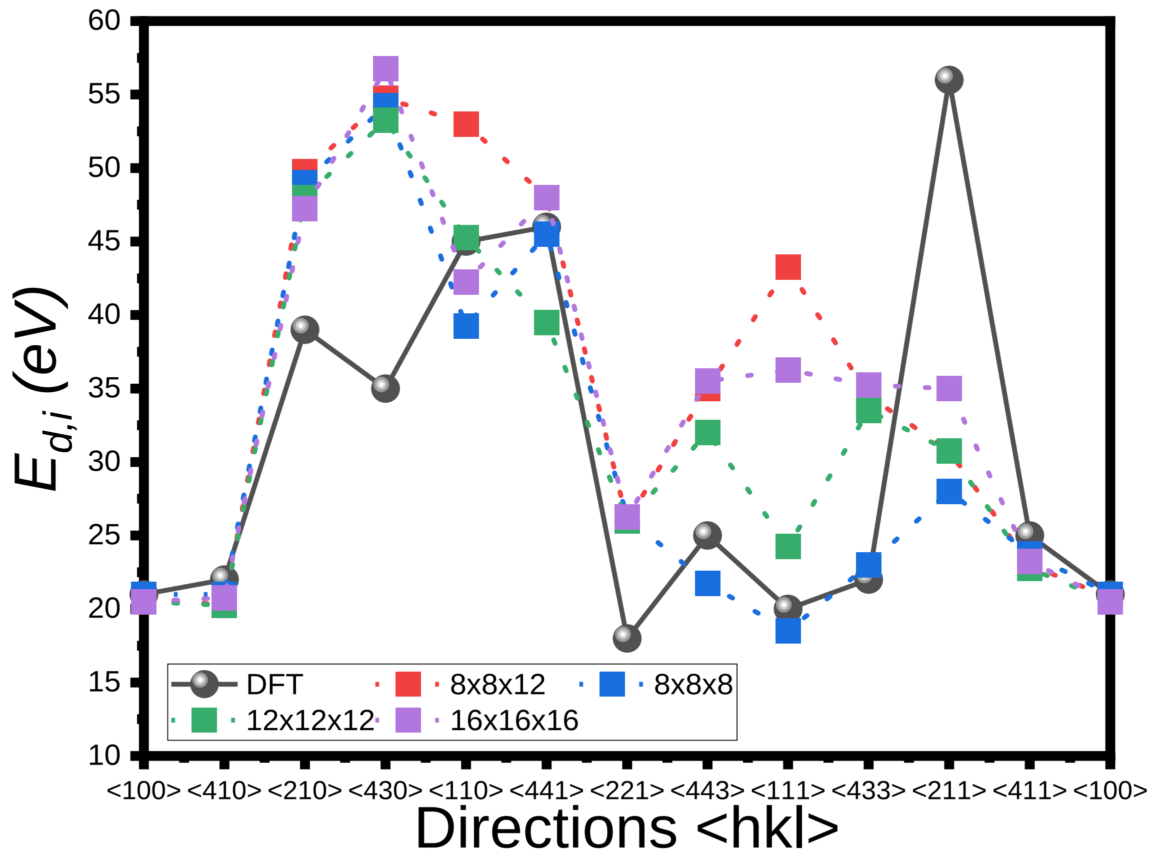


Fig. S2. Comparative study of the directional threshold displacement energy ($E_{d,i}$) of the current MD study with the DFT study form reference [4]. Among the examined structure the $E_{d,i\text{-}MD}$ with 8x8x8 supercell seems to be agrees with the major selective directions of $E_{d,i\text{-DFT}}$ values however the $E_{d,i\text{-}MD}$ over the <210>, <430> and <411> seems to be largely deviated from $E_{d,i\text{-DFT}}$ and this could be due to the potential shortcomings itself for estimating theses direction values.

Table S2. $E_{d,i}$ values for <111> direction with several supercells in the 0 K recoil simulation.

	8x8x8	**16x16x16**	**8x8x12**
<111>	18.5	36.25	43

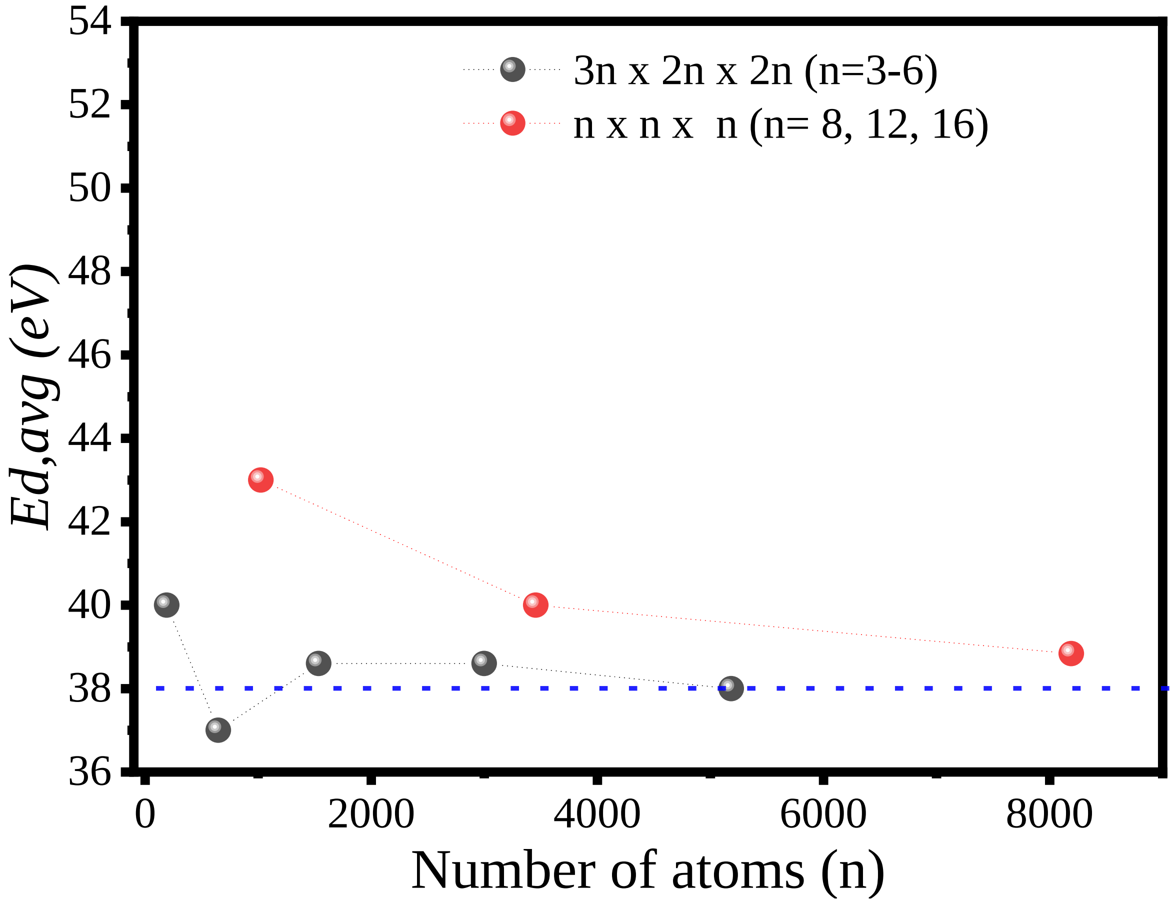


Fig.S3 the system shape and size effect on the $E_{d,avg}$ evaluation by MD.

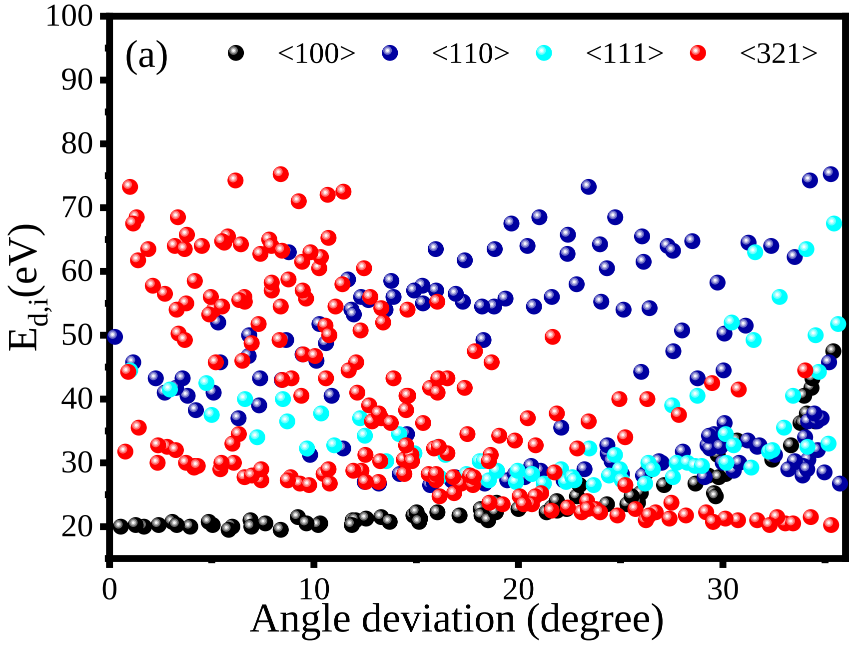


Fig. S4. The angle deviation of $E_{d,i}$ from the <100>, <110>, <111>, and <321> directions. The <100> shows the smoothest directional changes, which maintains at approximately 20 eV within 15° of deviation, while the other directions change largely. The <100> direction of $E_{d,i}$ has the most stable and the slowest deviation changes with angles up to 25°. In contrast, the $E_{d,i}$ for other directions change significantly even with slight degrees of deviation. We noted that the results agreed with the difficulties of $E_{d,i}$ evaluation for complex directions due to the large deviation in $E_{d,i}$ even with small angle changes.

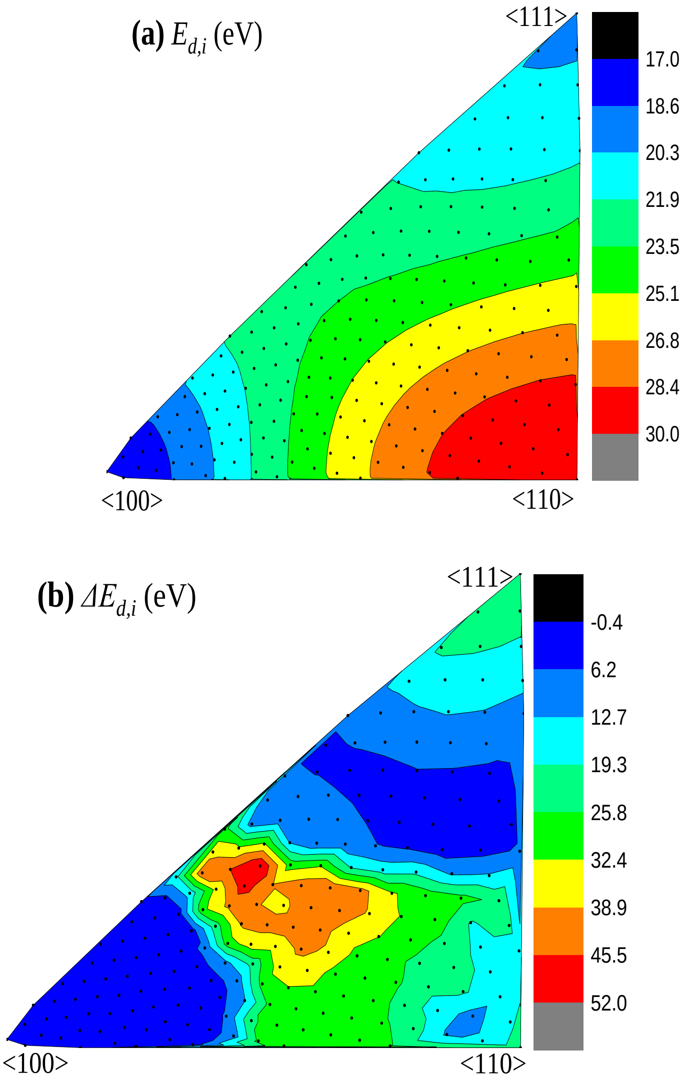
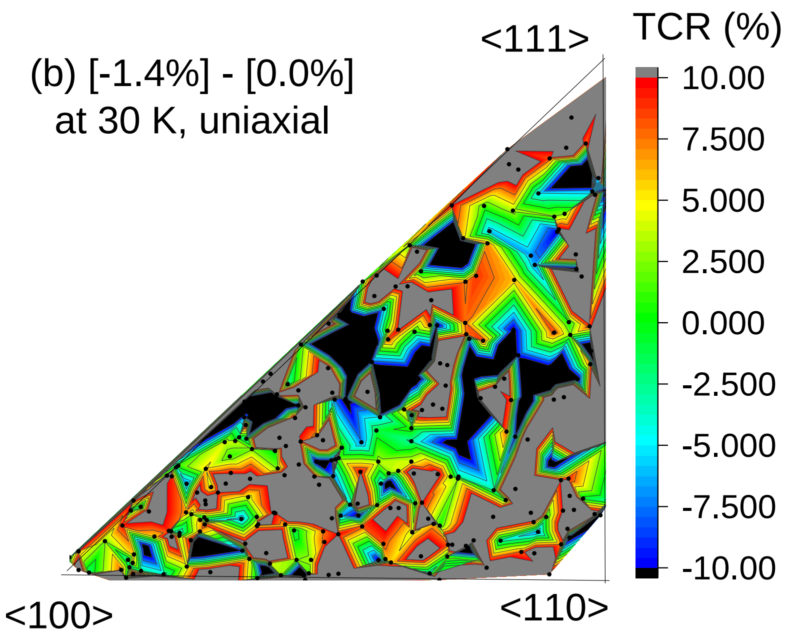


Fig. S5. (a) 210 ICD directions applied to generate 210 $\boldsymbol{E}_{\mathrm{d,i}}$ by applying the Seeger theoretical model.(b) The Seeger and the MD differences for $E_{\mathrm{d,i}}$ calculation ($\Delta E_{d,i} = E_{d,i,\text{ theory of each value of 210 ICD}} - E_{d,i,\text{ MD}}$).

The $E_{d,i}$ differences results between the theoretical and MD estimated values are shown in Fig. S5 (a),(b). Even though the distribution for <100> is consistent in both the theoretical and the MD evaluations, $E_{d,i}$ changes greatly for the <111> and <321>, which is why the theoretical model underestimates the $E_{d,i}$ and $E_{d,avg}$ values in the results, while overestimations are observed around the <111> direction up to 20 eV. The large contradiction between the results obtained by Seeger and our MD study is due to the limitation of the theoretical model, which is not sufficient to derive $E_{d,avg}$ from only three $E_{d,i}$ values. This is because an accurate value of directions as $E_{d,<110>}$ or $E_{d,<111>}$ are very difficult to obtain experimentally.



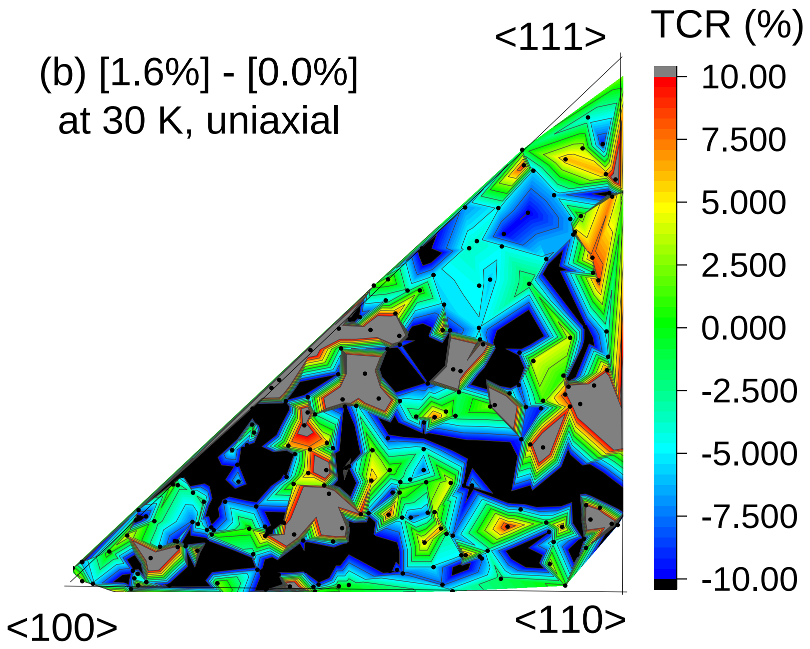


Fig. S6. The threshold displacement energy change rate (TCR) when structure deformed for 300 specific directions at 30 K. (a) is for uniaxial tensile strain and (b) is for uniaxial compression strain.

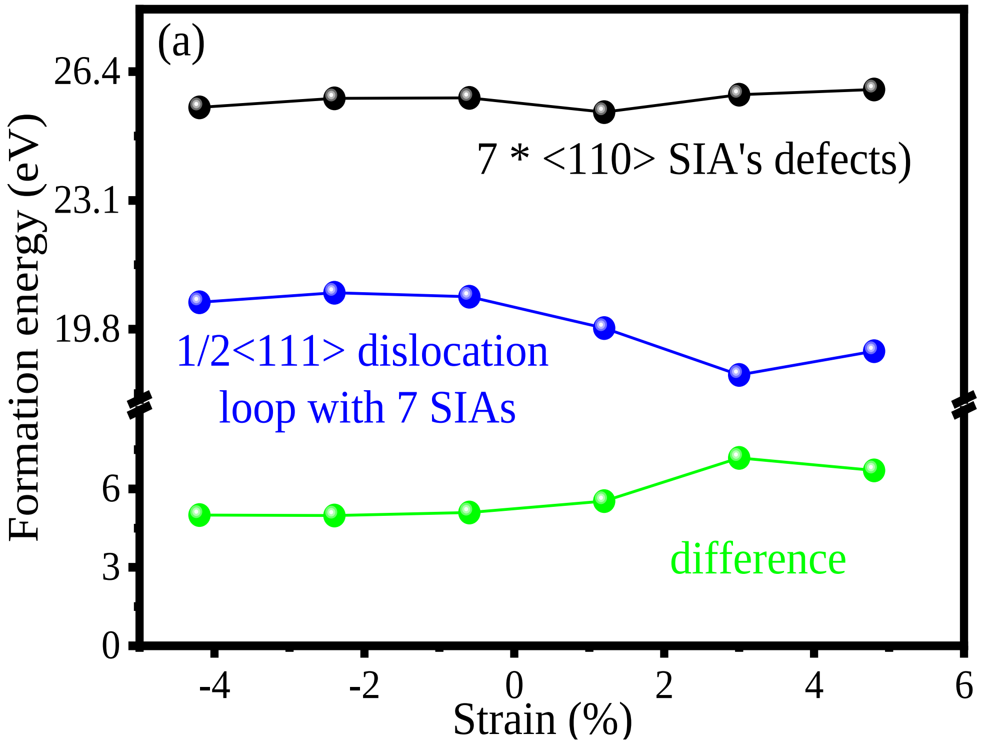


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Fig. S7. The formation energy of 1/2<111> dislocation loop with 7 SIAs and as compared with single <110> defects x 7. This graph when compared with the Fig. 6 (b) of the main manuscript we can see the dislocation formation is largely reduced by around 5 eV when tensile strain is applied.

References

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