

Supplementary materials

Influence of intrinsic strain on irradiation induced damage: the role of threshold displacement and surface binding energies

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Abstract

Supplementary materials for the article *Influence of intrinsic strain on irradiation induced damage: the role of threshold displacement and surface binding energies* from Julien Guénolé, Aruna Prakash and Erik Bitzek.

	Strain	Silicon			Aluminium	
		<i>As-cut</i>	<i>Recon.</i>	<i>Amorph.</i>	<i>As-cut</i>	<i>Amorph.</i>
E_{coh}	0 %	4.63	–	–	3.36	–
ΔH_S	0 %	4.5 - 5.2	–	–	3.2 - 3.5	–
SBE_k	0 %	4.73	–	–	3.19	–
SBE	-4 %	6.97 ± 0.01	10.57 ± 0.04	10.06 ± 1.06	4.47 ± 0.05	4.58 ± 0.43
	-2 %	6.97 ± 0.01	10.59 ± 0.03	10.04 ± 1.09	4.44 ± 0.05	4.60 ± 0.44
	0 %	6.97 ± 0.01	10.62 ± 0.02	10.03 ± 1.09	4.41 ± 0.05	4.60 ± 0.45
	+2 %	6.97 ± 0.01	10.64 ± 0.02	10.01 ± 1.08	4.36 ± 0.05	4.60 ± 0.45
	+4 %	6.93 ± 0.01	10.62 ± 0.02	9.97 ± 1.07	4.33 ± 0.05	4.60 ± 0.46

Table 1: Energies and surface binding energy for $\{001\}$ silicon and aluminium surfaces, in eV. E_{coh} , cohesive energy for the interatomic potentials used in the present work. ΔH_S , experimental energy of sublimation from [1] and [2]. SBE_k , surface binding energy from [3] based on the electronegativity concept. SBE, surface binding energy calculated in this work for different uniaxial tensile strains, as described in the text. The uncertainty is the sum of the standard deviation of the data set and the systematic error. It describes the spread of the SBE values.

References

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