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MDPI

Supplementary Materials

Bayesian Data Assimilation of Temperature Dependence of Solid–Liquid Interfacial Properties of Nickel

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Table S1. Representative properties of the EAM potential for Ni employed in this study [1,2].

Property	Experiment	EAM
Lattice constant, a_0 (nm)	0.352	0.352
Cohesive energy, e_0 (eV)	−4.45	−4.45
Elastic constants (GPa)		
B	181.0	181.0
c_{11}	246.5	241.3
c_{12}	147.3	150.8
c_{44}	124.7	127.3
Vacancy formation energy, E_v^f (eV)	1.60	1.57
Intrinsic stacking fault energy, γ_{SF} (mJ/m^2)	125	134
Symmetrical twin boundary energy, χ_T (mJ/m^2)	43	68
Surface energies (mJ/m^2)		
(110)	2280* (average)	2087
(100)	2280* (average)	1936
(111)	2280* (average)	1759

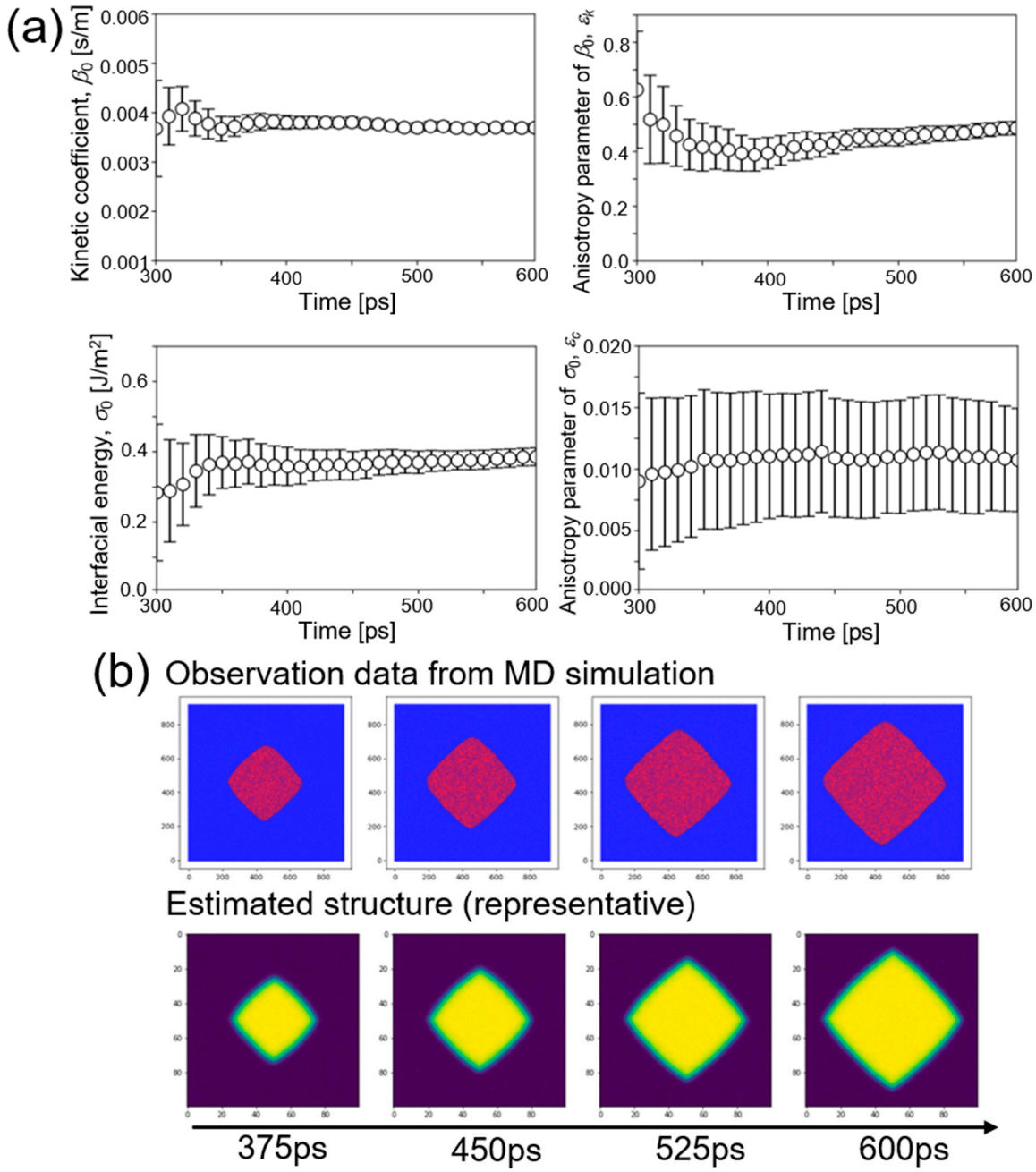

Figure S1. Estimation of four parameters (kinetic coefficient β_0, interfacial energy σ_0, and their anisotropy parameters ε_k and ε_c using observation data of molecular dynamics (MD) simulation at 1455 K. (**a**) Time changes of the estimated values of four parameters, β_0, σ_0, ε_k and ε_c. (**b**) Snapshots of observation data from MD simulation and representative result of estimated structure.

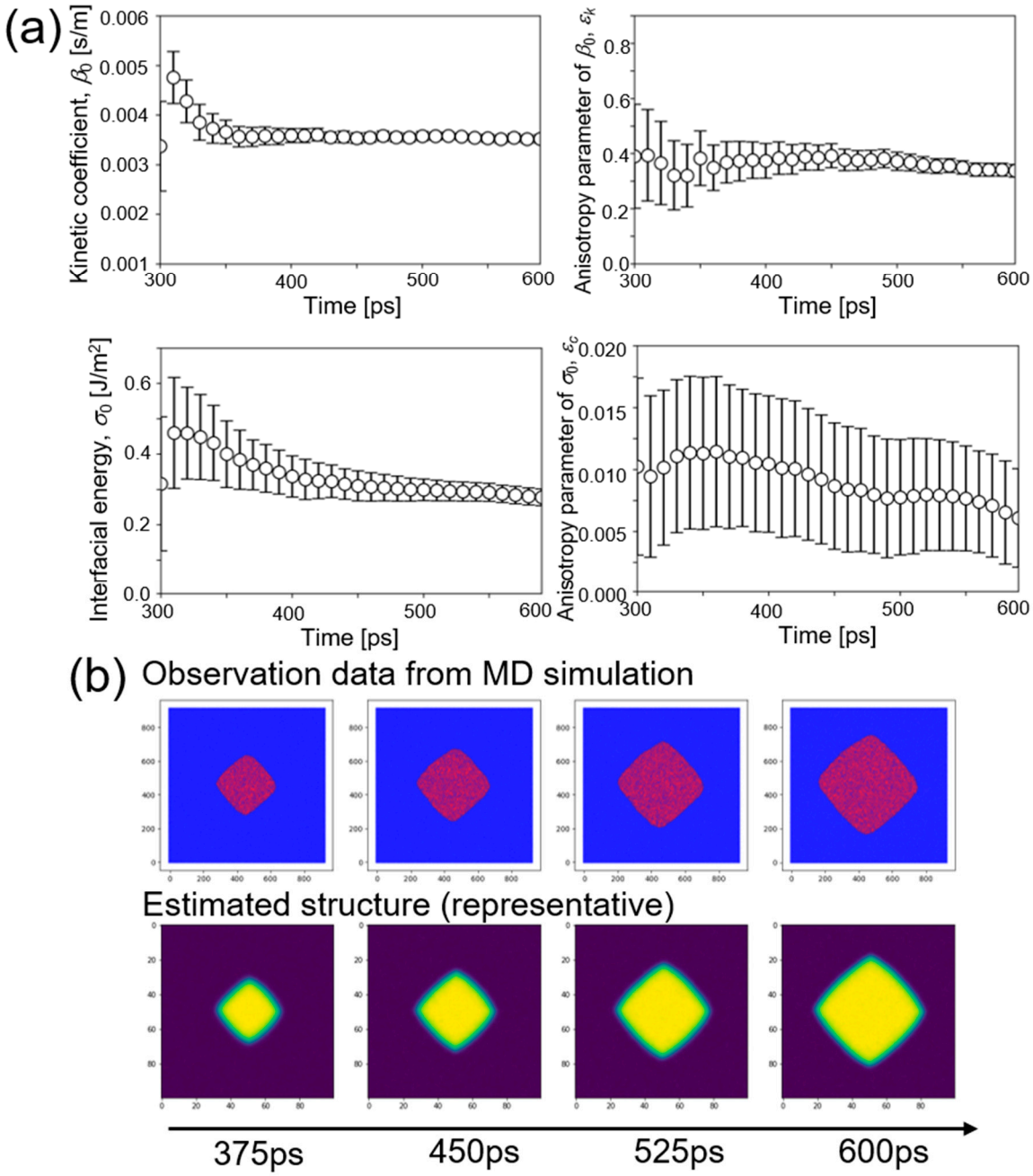

Figure S2. Estimation of four parameters (kinetic coefficient β_0, interfacial energy σ_0, and their anisotropy parameters ε_k and ε_c using observation data of molecular dynamics (MD) simulation at 1505 K. (**a**) Time changes of the estimated values of four parameters, β_0, σ_0, ε_k and ε_c. (**b**) Snapshots of observation data from MD simulation and representative result of estimated structure.

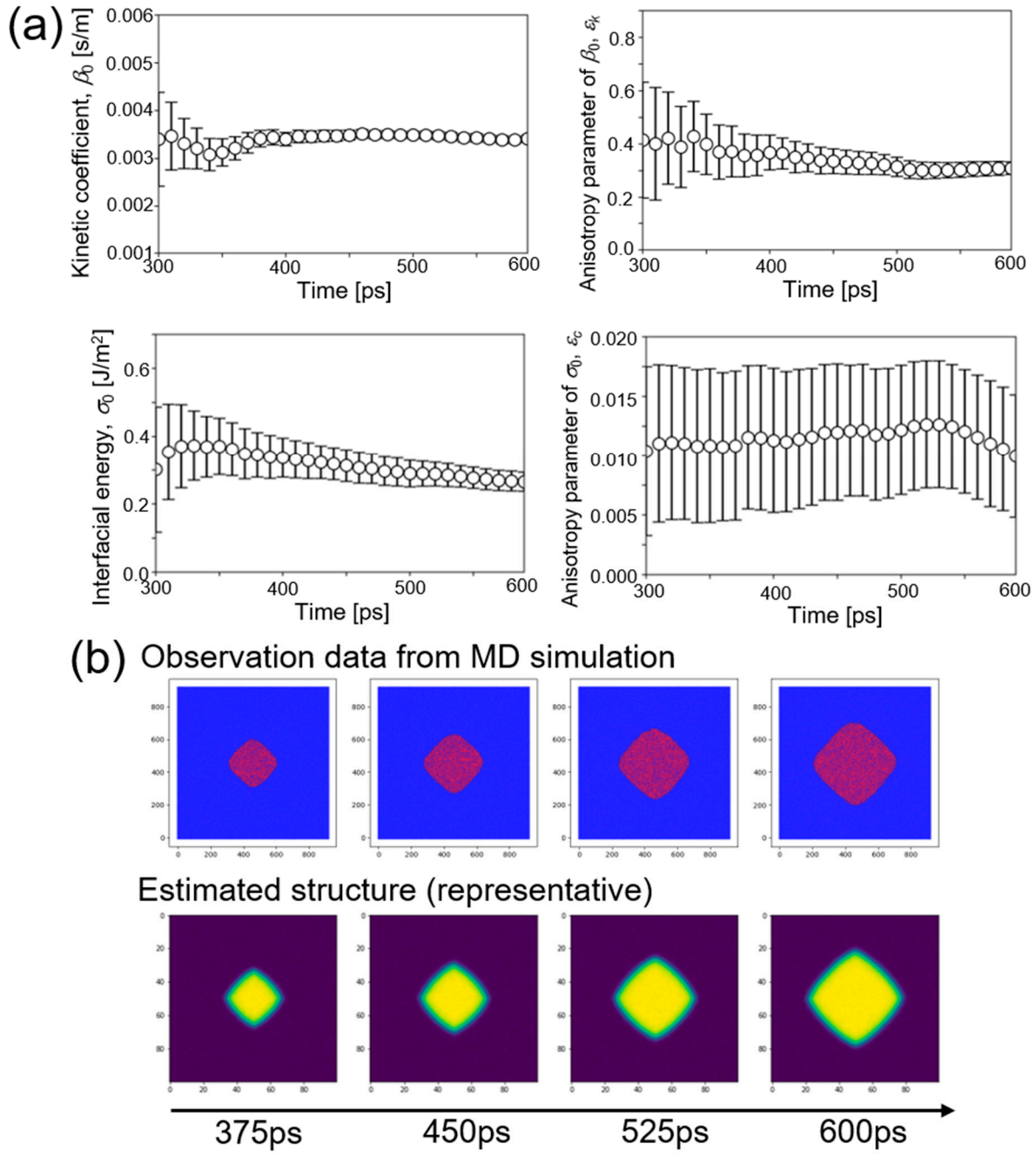

Figure S3. Estimation of four parameters (kinetic coefficient β_0, interfacial energy σ_0, and their anisotropy parameters ε_k and ε_c using observation data of molecular dynamics (MD) simulation at 1530 K. (**a**) Time changes of the estimated values of four parameters, β_0, σ_0, ε_k and ε_c. (**b**) Snapshots of observation data from MD simulation and representative result of estimated structure.

References

1. Purja Pun, G.P.; Mishin, Y. Development of an interatomic potential for the Ni-Al system. *Philos. Mag.* **2009**, *89*, 3245–3267.
2. Mishin, Y. Atomistic modeling of the γ and γ′-phases of the Ni–Al system. *Acta Mater.* **2004**, *52*, 1451–1467.