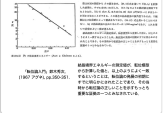


Stress

Energy

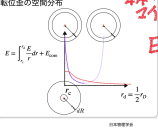
EAM fitted



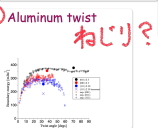
Model	Energy	Stress
POSCAR 10	...	...
POSCAR 11	...	...
POSCAR 12	...	...
POSCAR 13	...	...
POSCAR 14	...	...
POSCAR 15	...	...
POSCAR 16	...	...
POSCAR 17	...	...
POSCAR 18	...	...
POSCAR 19	...	...
POSCAR 20	...	...
POSCAR 21	...	...
POSCAR 22	...	...
POSCAR 23	...	...
POSCAR 24	...	...
POSCAR 25	...	...
POSCAR 26	...	...
POSCAR 27	...	...
POSCAR 28	...	...
POSCAR 29	...	...
POSCAR 30	...	...
POSCAR 31	...	...
POSCAR 32	...	...
POSCAR 33	...	...
POSCAR 34	...	...
POSCAR 35	...	...
POSCAR 36	...	...
POSCAR 37	...	...
POSCAR 38	...	...
POSCAR 39	...	...
POSCAR 40	...	...
POSCAR 41	...	...
POSCAR 42	...	...
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POSCAR 44	...	...
POSCAR 45	...	...
POSCAR 46	...	...
POSCAR 47	...	...
POSCAR 48	...	...
POSCAR 49	...	...
POSCAR 50	...	...
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POSCAR 52	...	...
POSCAR 53	...	...
POSCAR 54	...	...
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POSCAR 56	...	...
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POSCAR 58	...	...
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POSCAR 69	...	...
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POSCAR 74	...	...
POSCAR 75	...	...
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POSCAR 77	...	...
POSCAR 78	...	...
POSCAR 79	...	...
POSCAR 80	...	...
POSCAR 81	...	...
POSCAR 82	...	...
POSCAR 83	...	...
POSCAR 84	...	...
POSCAR 85	...	...
POSCAR 86	...	...
POSCAR 87	...	...
POSCAR 88	...	...
POSCAR 89	...	...
POSCAR 90	...	...
POSCAR 91	...	...
POSCAR 92	...	...
POSCAR 93	...	...
POSCAR 94	...	...
POSCAR 95	...	...
POSCAR 96	...	...
POSCAR 97	...	...
POSCAR 98	...	...
POSCAR 99	...	...
POSCAR 100	...	...

鈴木秀次先生の記述  
転位論入門  
(マクネ, 67)

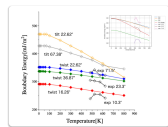
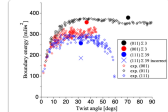
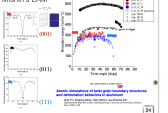
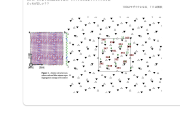
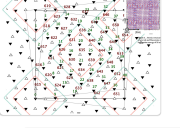
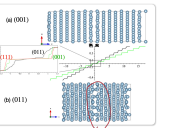
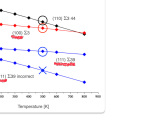
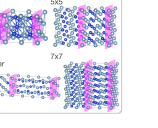
(T.M.)<sup>2</sup>  
森 勉 山 村 外 志 夫  
新 刊 物 社  
Eigen 歪



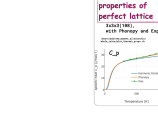
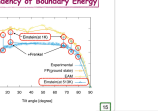
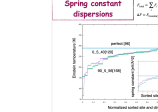
① Al 傾角 有限 温度  
Finite temperature boundary energy of Al  
A. 1000, symmetric fit



② Aluminum twist ねじり?



Where is wrong?  
Reason of failure on boundary energies  
Global relaxation?  
Too small model?  
Potential?  
Temperature effect?  
MDP apps with small models  
on Al (100) symmetric fit  
finite temp. (not phonon)



Where is the error?  
As(100) symmetric fit boundary energy with VASP  
Small model:  
GK by Boettger method  
Ornstein-Zernike (OZ)  
isB1 wrong  
Einstein model:  
incompatible with Experimental results  
Frenkel method:  
thermal effect of anharmonicity

