分子动力学算例

GSF曲线及单晶NT Cu的单轴拉伸

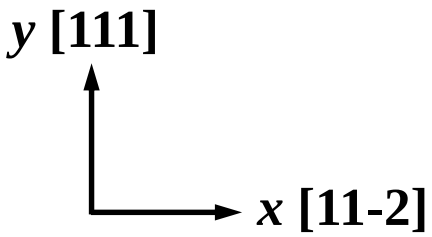
2021年1月12日

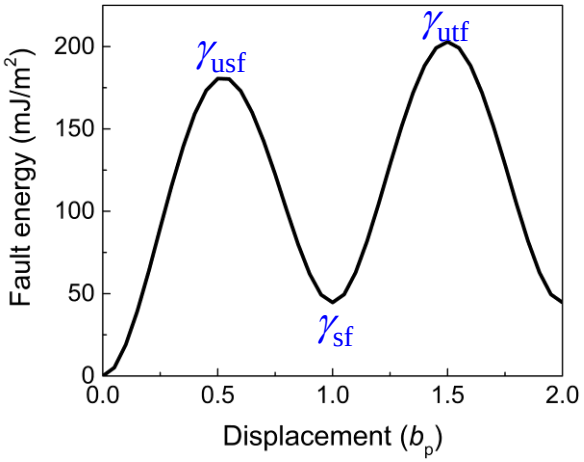
GSF曲线计算（Cu）

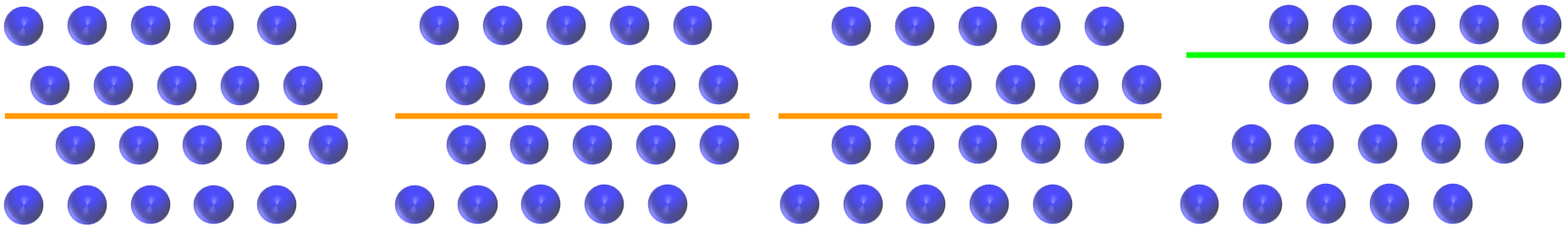
GSF曲线

$\boldsymbol{b}_p = a_0$ [11-2]/6

$b_p = a_0 / 6^{1/2}$

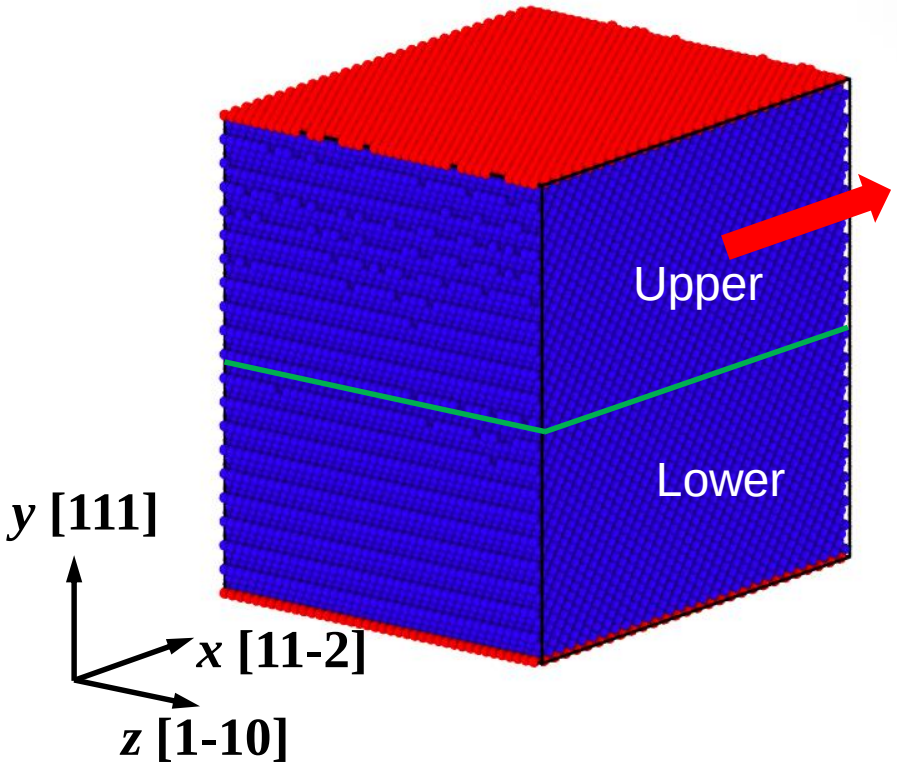




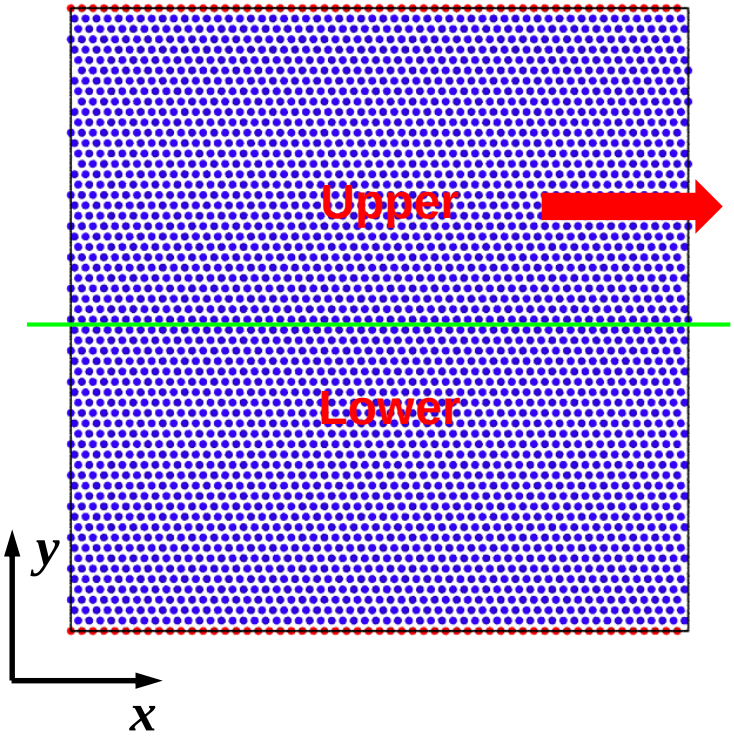


	γ_{usf}	γ_{sf}	γ_{utf}
Perfect FCC	0.5 $\boldsymbol{b}_p$	$\boldsymbol{b}_p$	1.5 $\boldsymbol{b}_p$
	Unstable stacking fault	**Stable stacking fault**	**Untable twin fault**

GSF曲线计算（Cu）

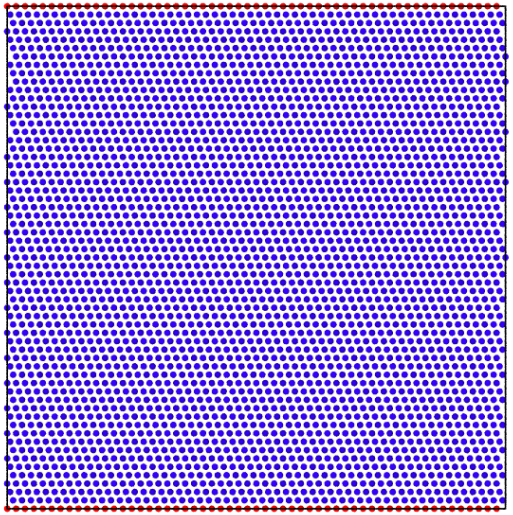


- 模型尺寸：12.4×12.5×10.2 nm^3
- 势函数：EAM (Mishin Y, et al., Phys. Rev. B, 2001)
- *x*, *z* 方向周期性边界条件
- *y* 自由边界条件

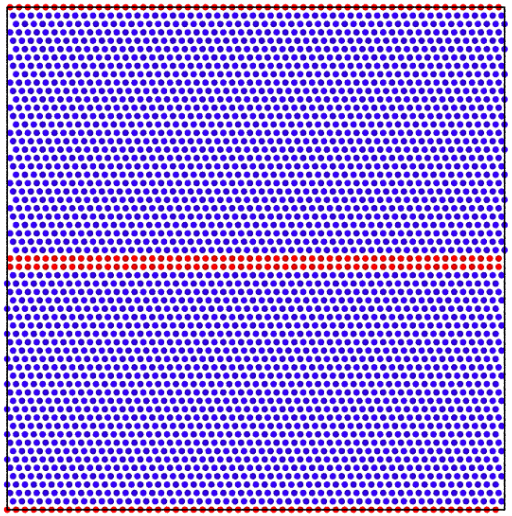



```
label forloopp
variable a loop 20
variable p equal "v_partial/20"
displace_atoms up1 move ${p} 0 0 units box
variable gsf equal "(v_gbenergy-v_gbenergy0)/lx/lz*16.02*1000"
fix extra all print 1 "$a  ${gsf}" append gsfe_Cu.txt screen no
run 1
next a
jump gsf.in forloopp
```

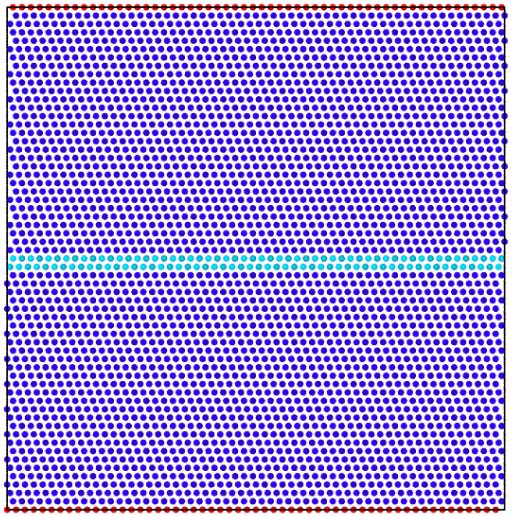
GSF曲线计算 （Cu）



初始结构

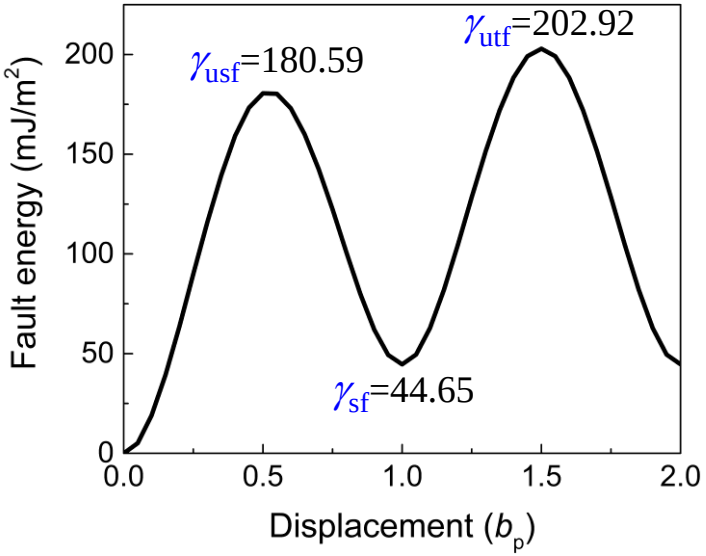


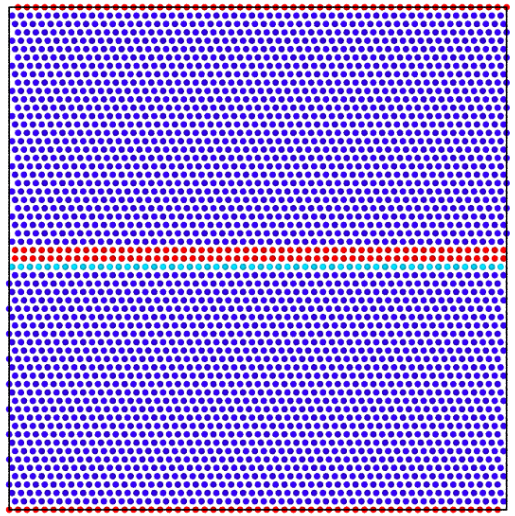
0.5 $\boldsymbol{b}$p



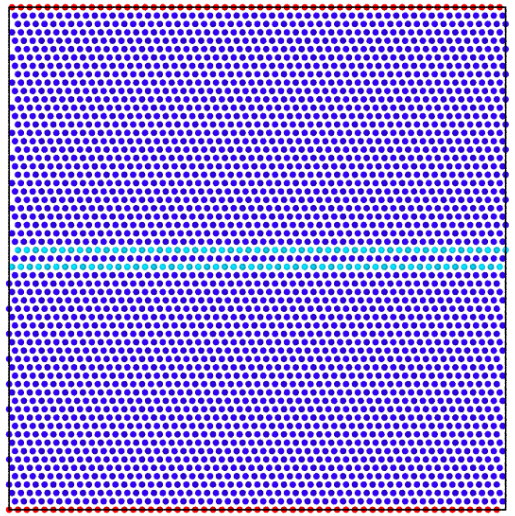
$\boldsymbol{b}$p

GSF曲线





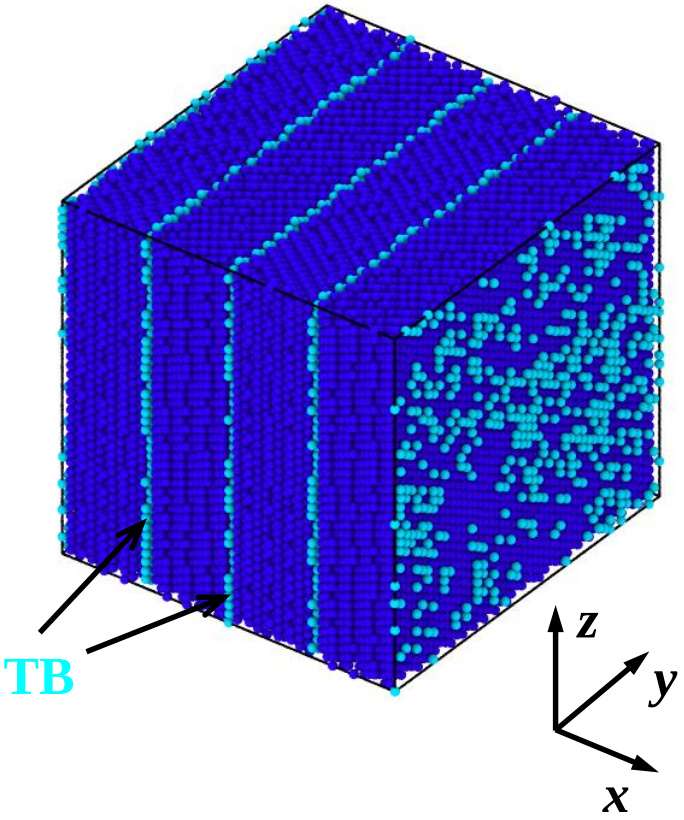
1.5 $\boldsymbol{b}$p



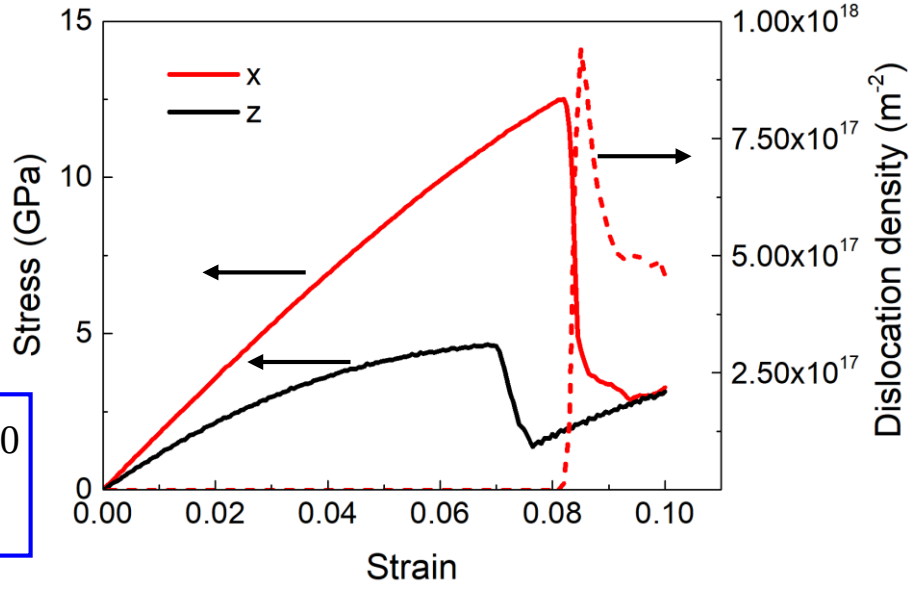
2.0 $\boldsymbol{b}$p

单晶纳米孪晶Cu的拉伸模拟

原子模型



- 模型尺寸：10.0×10.6×10.2 nm^3
- 孪晶厚度：2.5 nm
- 边界条件：周期性边界条件
- 势函数：EAM (Mishin Y, Phys. Rev. B, 2001)
- 系综：NPT
- 温度：300 K
- 拉伸方向 *x* <111>, *z* <110>
- 应变率： $5\times10^{8}\ s^{-1}$




```
fix 1 all npt temp 300.0 300.0 0.1 y 0.0 0.0 1.0 z 0.0 0.0 1.0
fix 2 all deform 1 x erate 0.0005 units box remap x
```