Kinetics of ordering and metastable phase of alloys

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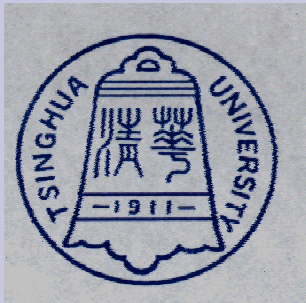

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References

- L. Shi and J. Ni, Phys. Rev. Lett. 97, 126105 (2006).
- Z. Q. Liu and J. Ni, J.Phys.: Condens. Matter 17, 5355 (2005).
- L. Shi and J. Ni, Phys. Rev. B 69, 155428 (2004).
- L. Shi, H. T. Shi, and J. Ni, Comp. Materials Science 30, 326-330 (2004).

Main Contents

- Introduction
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- Kinetics of ordering during alloy film growth
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Introduction

- Non-equilibrium growth: rapid quench, laser treatment, ion bombartment, and various epitaxial growth methods for the growth of materials in non-equilibrium state and metastable state.
- It is important to understand the basic kinetic processes during the growth. The equilibrium phase diagrams can not deliver enough information on non-equilibrium growth.

Methods

Kinetic process

- PPM method
- Master equation method
- Monte-Carlo method

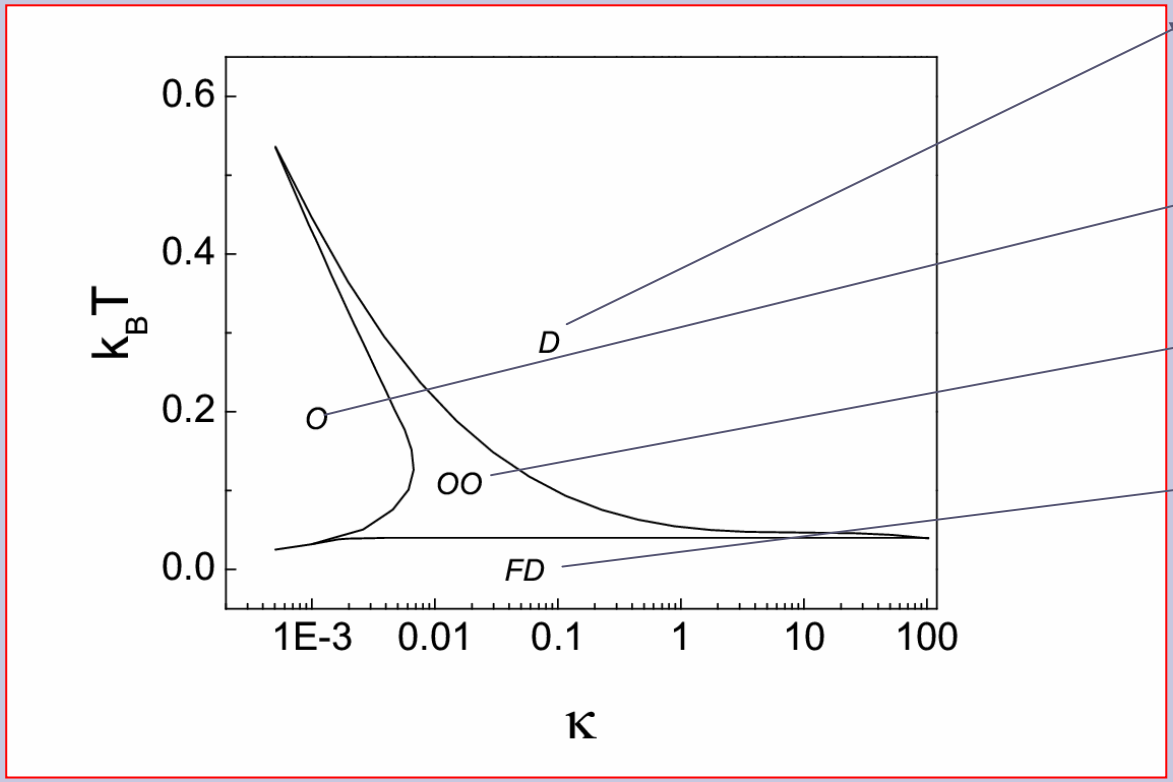
Energy parameters

- First principle methods

Introduction

- Epitaxial growth (MBE、MOCVD): layer by layer growth.
- Fcc ordering: Ordering structures in metal alloys: CuAu; CoPt; FePt;
- Ⅲ-Ⅴ semiconductor alloys,

Kinetical phase diagram



Disordered phase

Equililbrium ordered phase

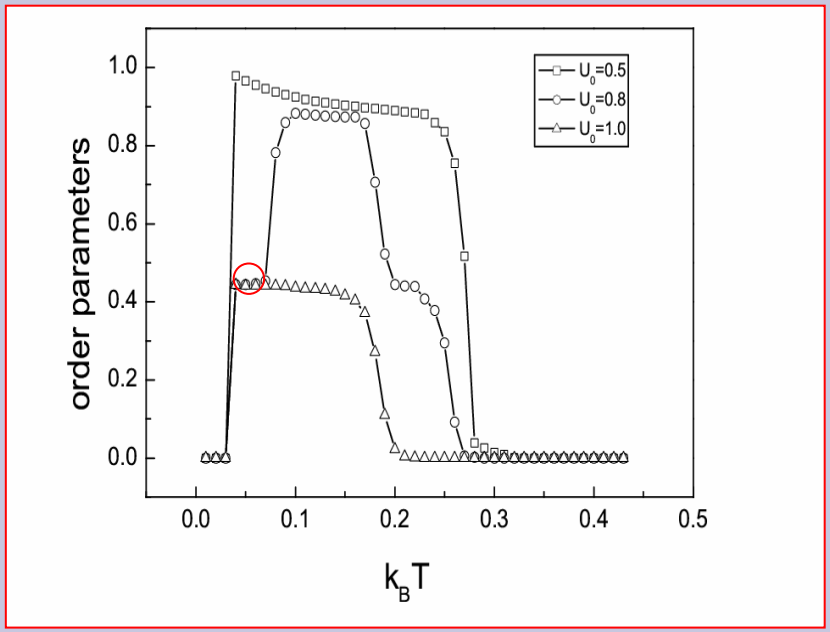
Oscillated ordered phase

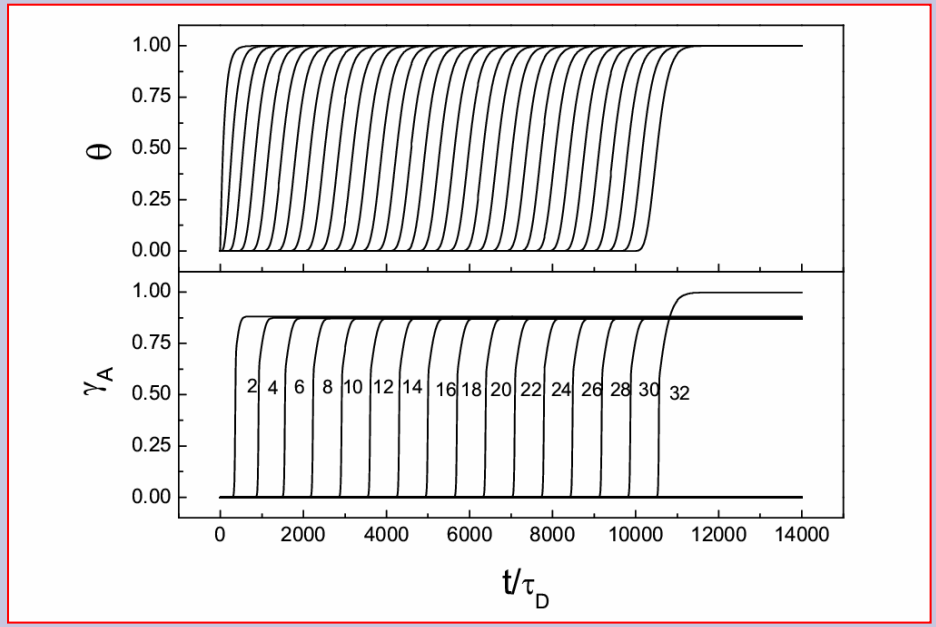
Quenched disordered phase

Phase diagram with temperature and ratio κ as parameters

$$U_0 = 1.0, \quad \mu_A = \mu_B = 0.25, \quad P_A^{\alpha} = P_A^{\beta} = 1.0, J = 1$$

Oscillated ordering

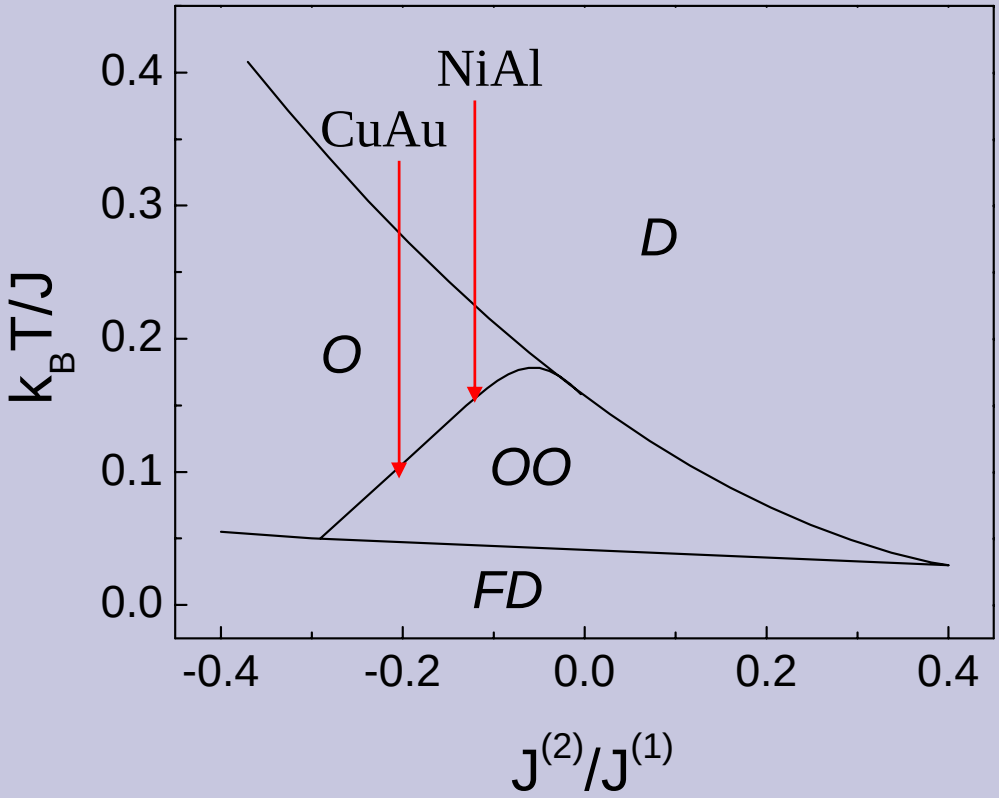




Kinetical induced oscillated ordering

$$k_BT/J=0.06,\quad \kappa=5\times10^{-3},\quad U_0=0.8,\quad \mu_A=\mu_B=0.25,\quad P_A^{\alpha}=P_A^{\beta}=1.0$$

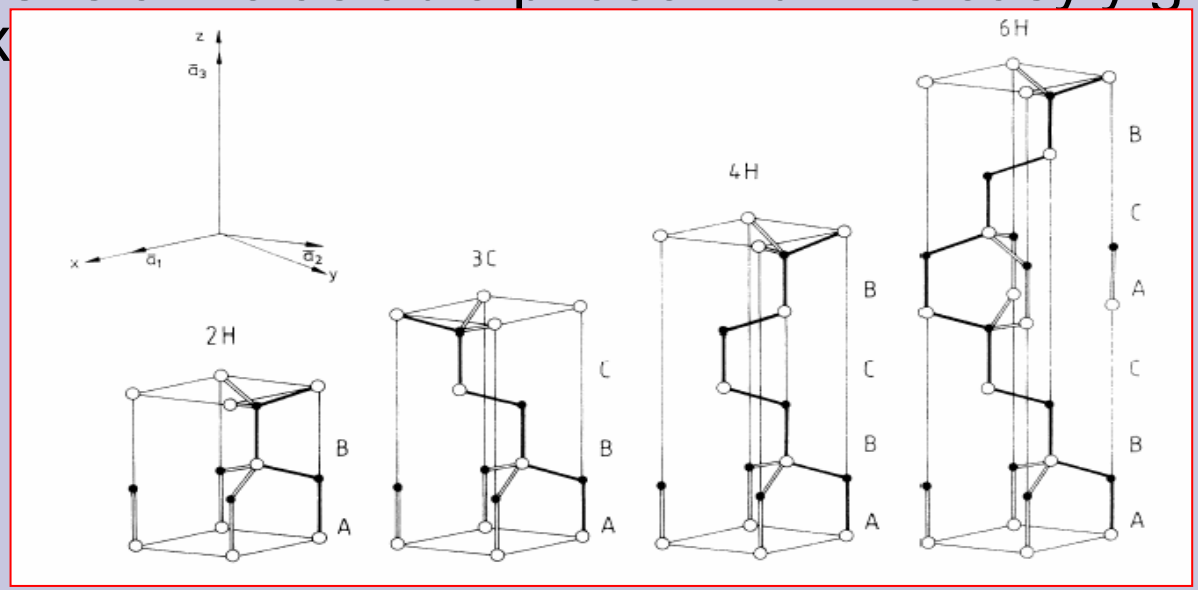
Nearest neighbor interaction



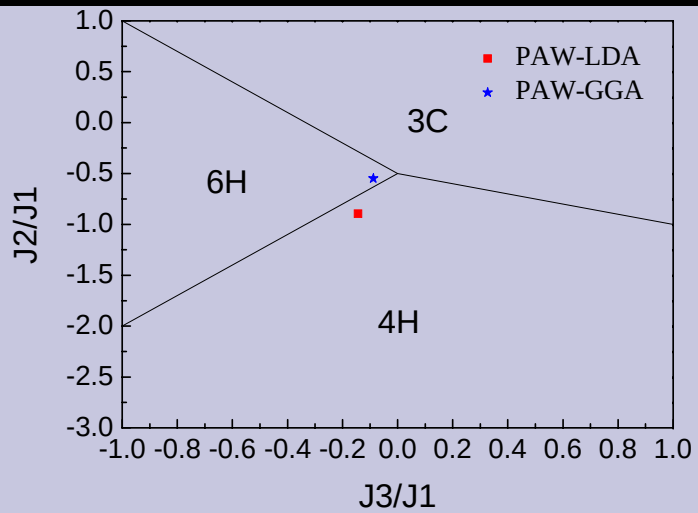
$\kappa = 5\times10^{-3}, \quad U_0 / J = 1.0, \quad \mu_A = \mu_B = 0.025eV$

Kinetic phase diagrams of epitaxial growth for SiC polytypes

- The most common polytypes are zinc-blende SiC (3C-SiC), wurtzite SiC (2H-SiC), 4H-SiC,6H-SiC, and 15R-SiC.
- The origin of polytypism in SiC is still not completely understood. The polytypes should be viewed as the non-equilibrium structures arising from special growth mechanisms
- 3C-SiC is a metastable phase. But it is easyly grown by epitax

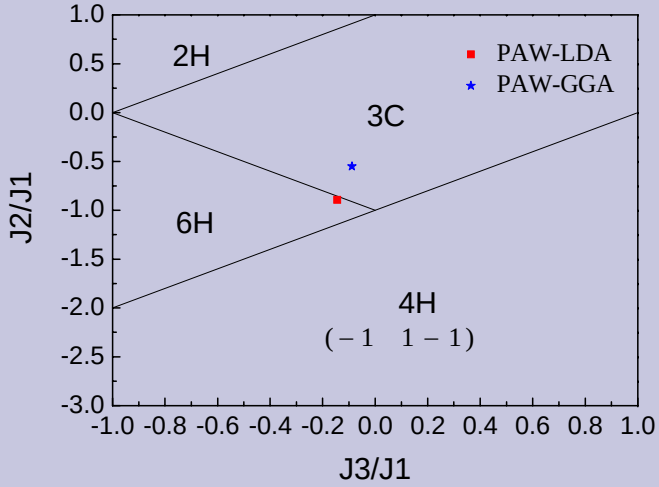


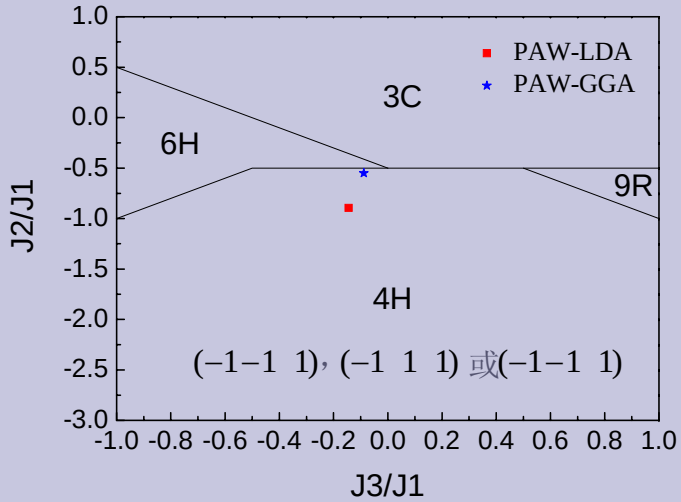
Kinetic phase diagrams of SiC epitaxial growth



Phase diagram of ground states

Z. Q. Liu and J. Ni, J.Phys.: Condens. Matter 17, 5355 (2005).

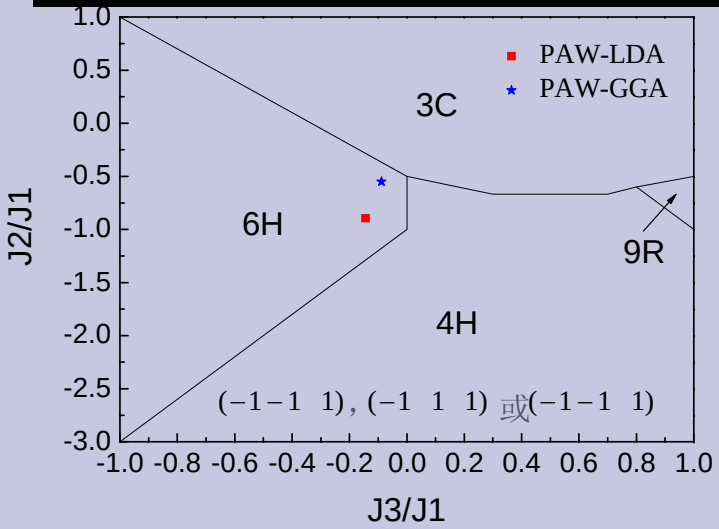




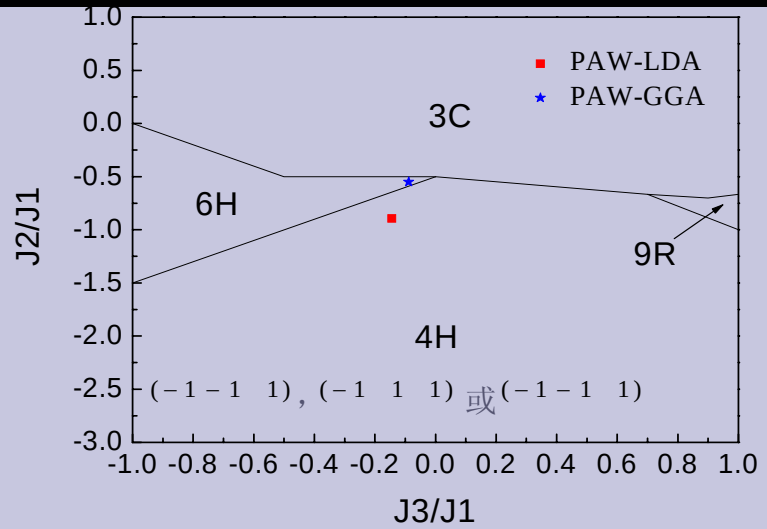
the rearrangement of atoms in one surface bilayer is allowed

the rearrangement of atoms in two surface bilayer is allowed

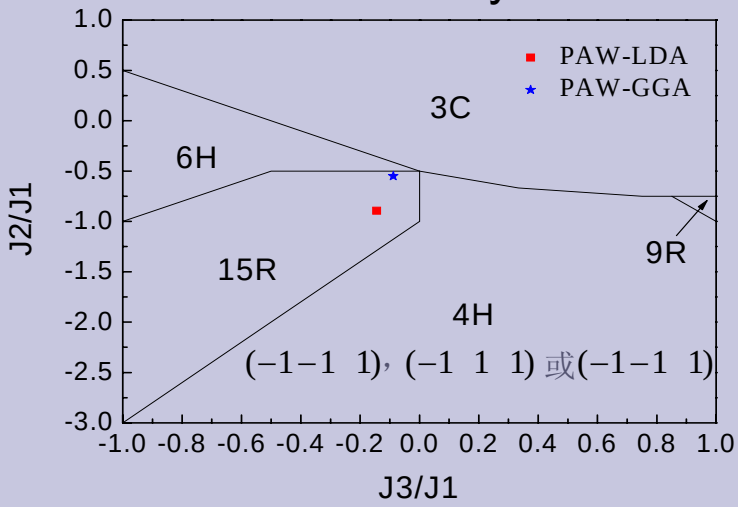
Kinetic phase diagrams of SiC epitaxial growth



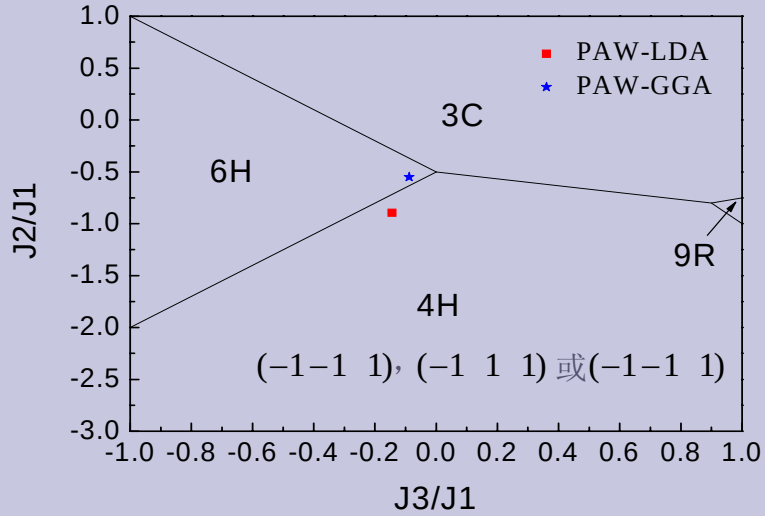
the rearrangement of atoms in three surface bilayer is allowed



the rearrangement of atoms in four surface bilayer is allowed



the rearrangement of atoms in



the rearrangement of atoms in six

surface bilayer is allowed

The CoPt alloy films

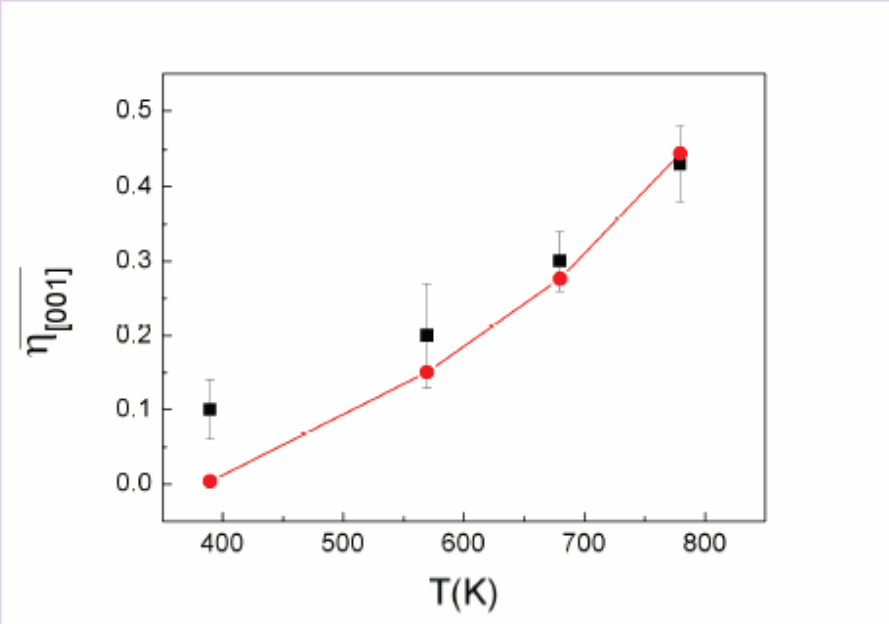
1. We consider an fcc film of CoPt alloy grown in the [001] direction on the buffer layer is Pt layer
2. The order parameter in the [100] direction is: $\eta_{[100]}(m) = P^{\alpha}_{Co}(m) - P^{\beta}_{Co}(m)$
3. The order parameter in the [001] direction is: $\eta_{[001]}(m) = |x_{Co}(m) - x_{Pt}(m)|$
4. the total energies of structures calculated by VASP.

- The kinetic equations of growth consist of all the three contributions from the diffusion, evaporation, and adsorption processes

$$\frac{dP^s_i(m)}{dt} = \sum_j \sum_{s'} (Y^{ss'}_{ji} - Y^{ss'}_{ij}) + Z^s_i(m) + X^s_i(m)$$

Ordering of the CoPt alloy films

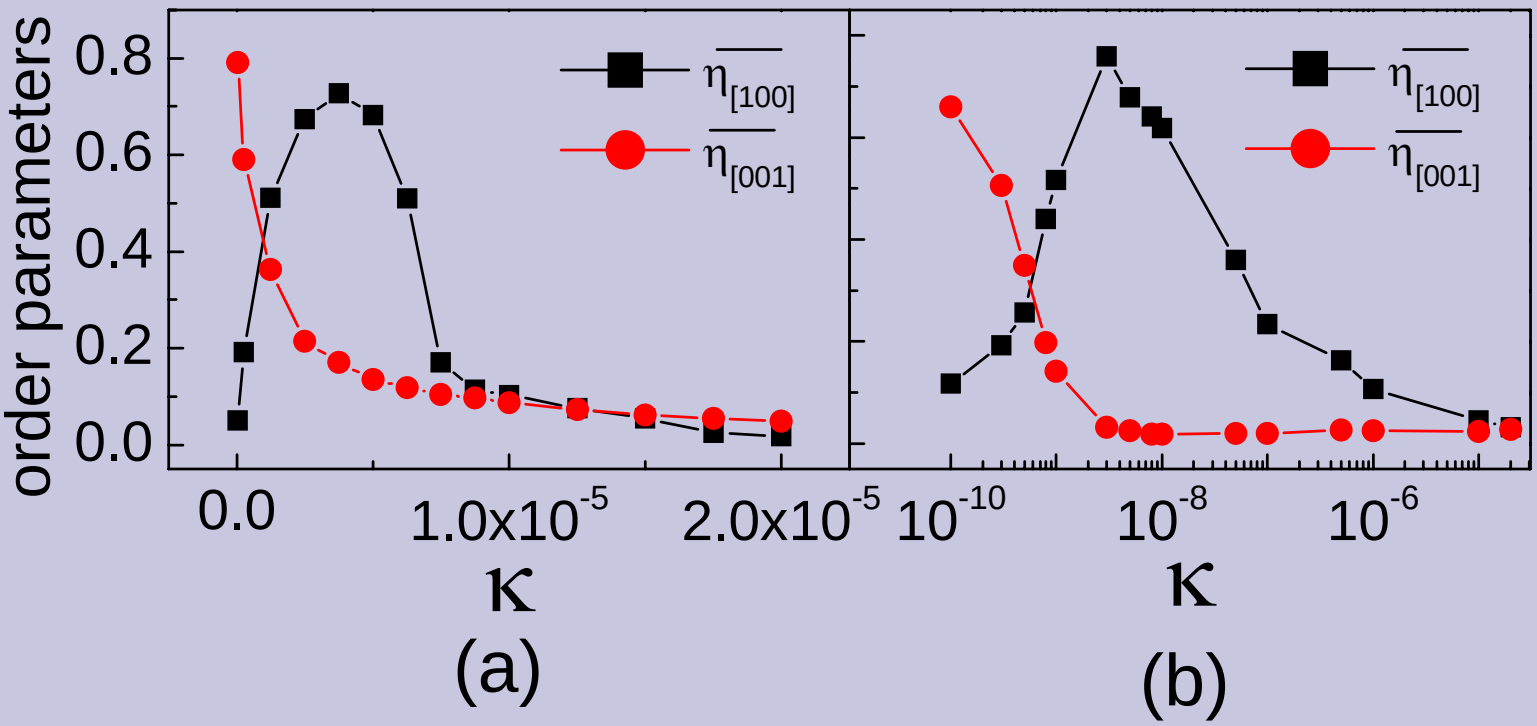
The experiment result and simulation result:



The average order parameter in the [001] direction as a function of temperature with $\kappa = 5.0 \times 10^{-6}$, where square dots are the experiment data.

(O. Ersen, et al J. Appl. Phys. 93, 2987 (2003).)

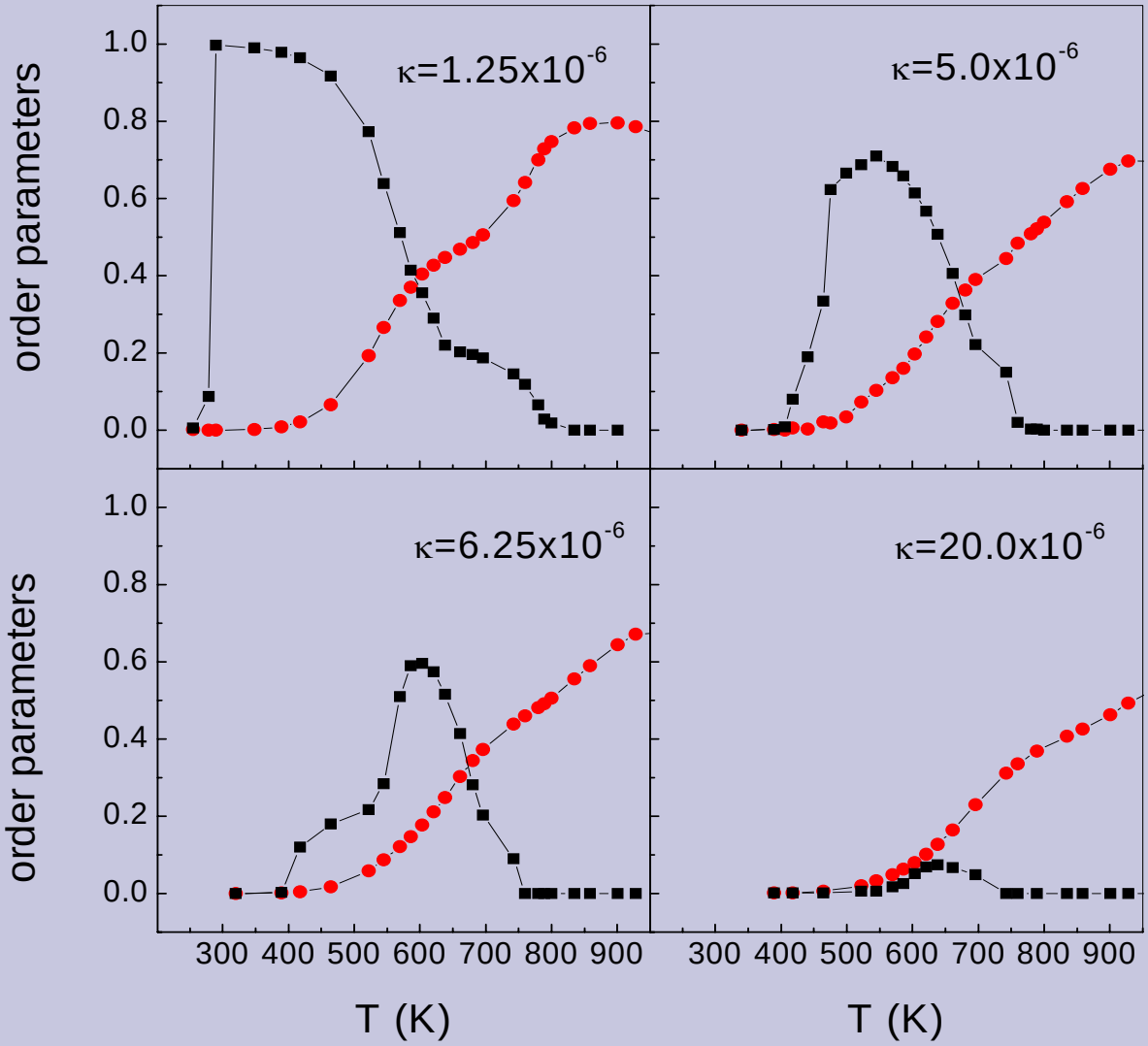
Variation of order parameters with the increase of growth rate



- The average order parameters of 8 layer films as a function of & with T=570 K

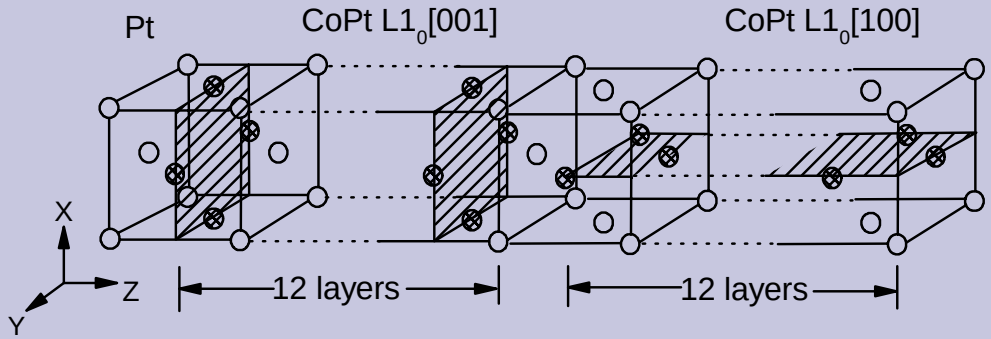
- L. Shi and J. Ni, Phys. Rev. Lett. 97, 126105 (2006).

Variation of order parameters with temperature

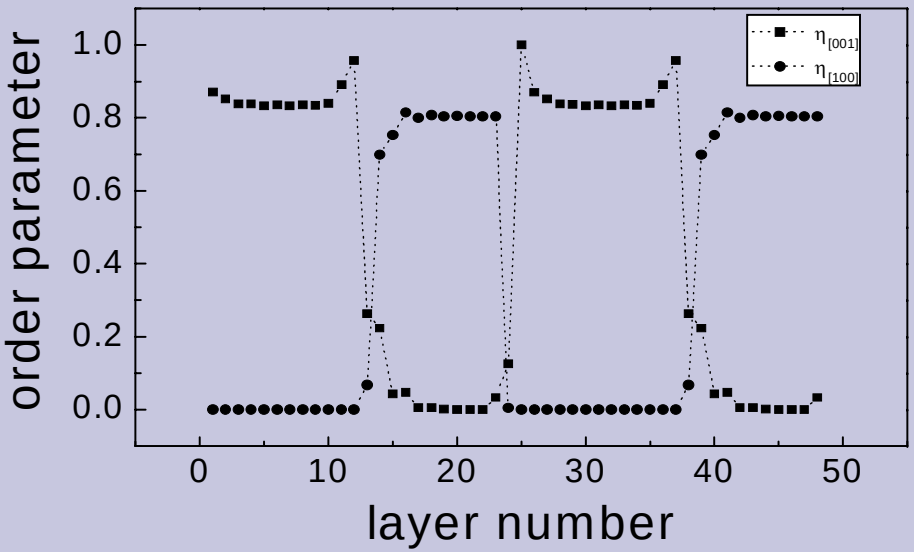


- The average order parameters of 8 layer films as a function of temperature

Ordering orientation superlattice



(a)



(b)

- (a) The superlattice with the ordering-orientation transition per 12 layers. (b) The order parameters of the ordering orientation superlattice.

- L. Shi and J. Ni, Phys. Rev. Lett. 97, 126105 (2006).

Summary

- Kinetics of ordering in alloy films and Kinetic phase diagrams, there is an oscillated ordered phase with occurrence conditions of high deposition rate
- The 3C-SiC phase would grow epitaxially in low temperature. The 4H-SiC phase would grow epitaxially in intermediate temperature. The 6H-SiC or 15R-SiC phases would grow epitaxially in higher temperature.This is in agreement with experiments
- We have investigated the effect of the kinetic anisotropy on the formation of structures in the epitaxial growth of alloy films. the ordering orientation of the $L1_0$ ordered structure changes from the [001] direction to the [100] direction with the increase of the growth rate.
- We propose a simple method to synthesize the ordering orientation surperlattice by periodically changing the growth rate.

Thank You

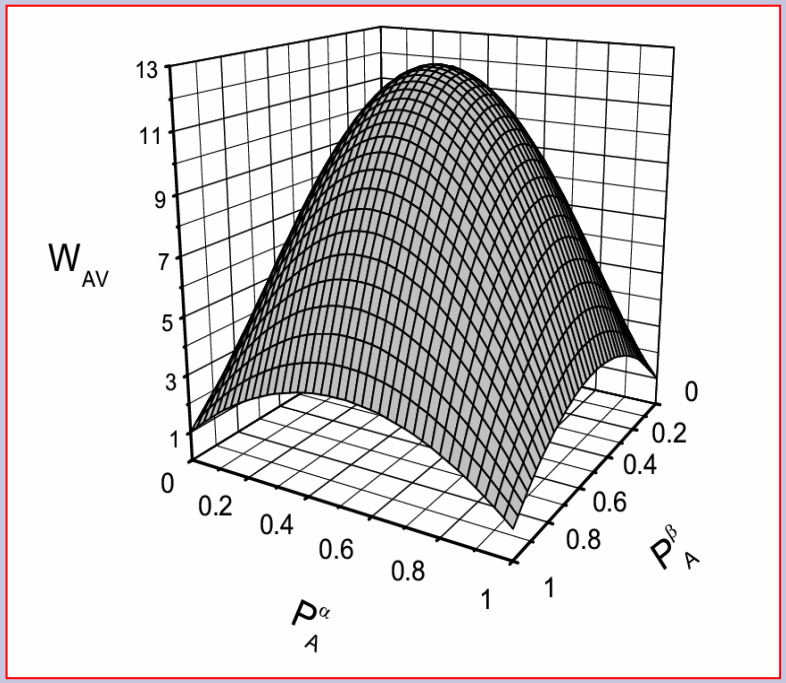
Master equation method

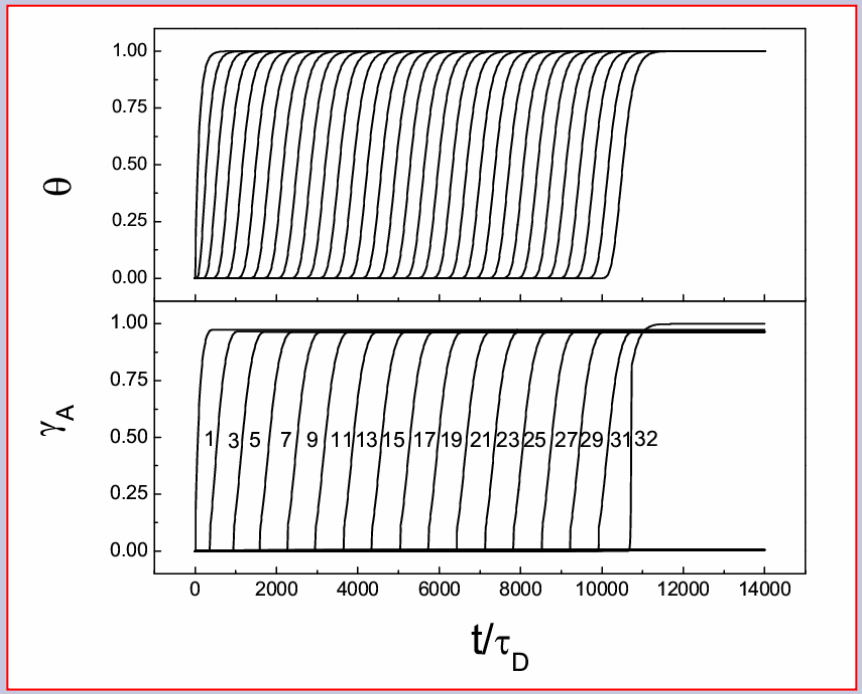
- Master equation method

$$\frac{d}{dt}P_{\alpha_i}(\vec{r}_i,t)=\sum_{j\neq i}\sum_{\{x\}}R_{\alpha_j,\alpha_i,\{x\}}(\vec{r}_i,\vec{r}_j,\{\vec{x}\})P_{\alpha_j,\alpha_i,\{x\}}(\vec{r}_i,\vec{r}_j,\{\vec{x}\})$$
$$-\sum_{j\neq i}\sum_{\{x\}}R_{\alpha_i,\alpha_j,\{x\}}(\vec{r}_i,\vec{r}_j,\{\vec{x}\})P_{\alpha_i,\alpha_j,\{x\}}(\vec{r}_i,\vec{r}_j,\{\vec{x}\})$$

- $P_{\alpha 1,\ldots,\alpha n}(r_1,\ldots,r_n;t)$: cluster probability
- $R_{\alpha 1,\ldots,\alpha n}(r_1,\ldots,r_n;t)$: exchange rate.
- {x}: neighboring cluster of interacting neighborhood.

Oscillatory ordered phase



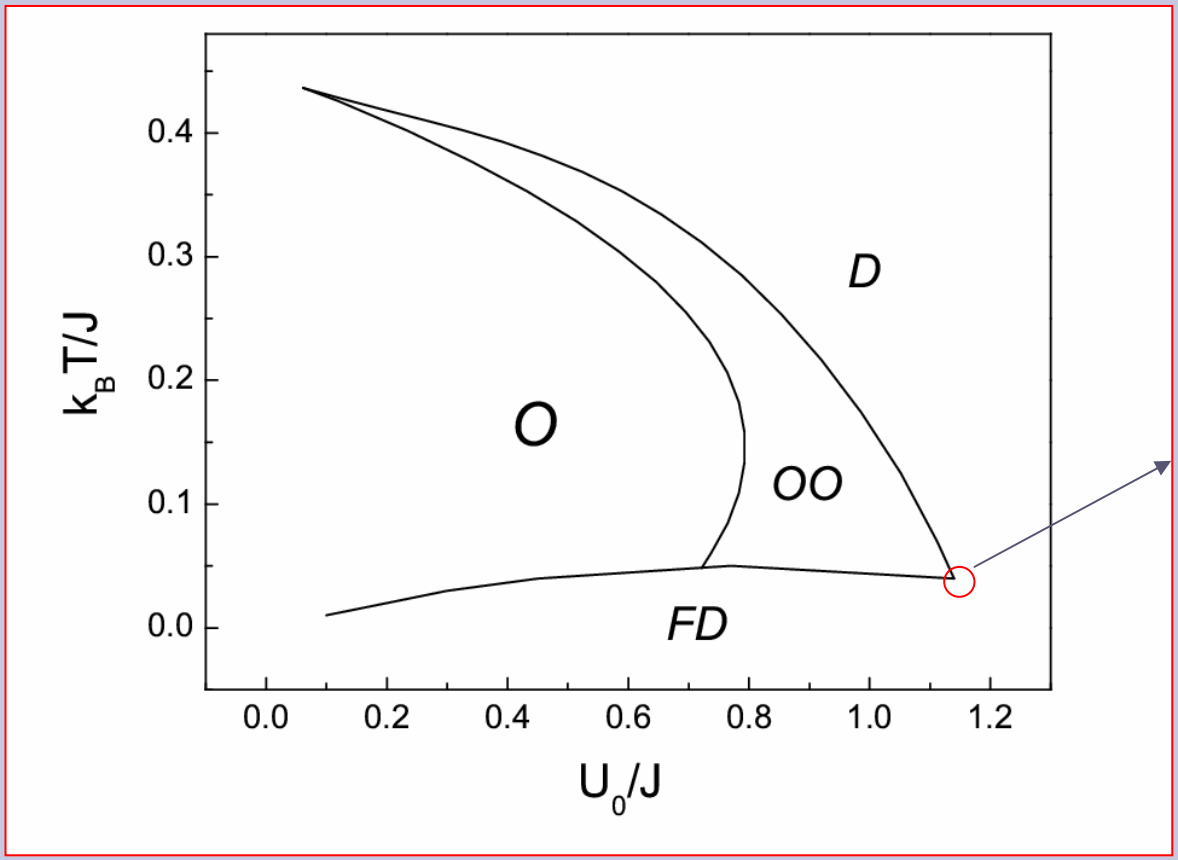


- Effects of underlayer on the broken factor

Ordering in the odd layers

$$k_B T / J = 0.06, \quad \kappa = 5\times10^{-3}, \quad U_0 = 0.8, \quad \mu_A = \mu_B = 0.25, \quad P_A^{\alpha} = P_A^{\beta} = 0.5$$

Kinetic phase diagram



Phase diagram with temperature and energy barrier as parameters

$\kappa = 5\times10^{-3}, \quad \mu_A = \mu_B = 0.25, \quad P_A^{\alpha} = P_A^{\beta} = 1.0$