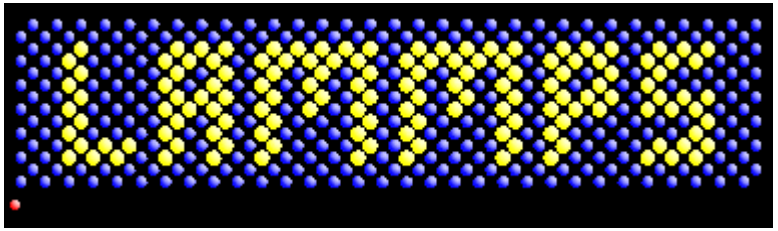
12月7日上机实习安排

LAMMPS软件中ReaxFF力场的使用：

1. 自行安装LAMMPS软件的Windows版本
2. Reactive mechanism investigation of nickel-catalyzed transformation of amorphous carbon (*a*-C) into graphene rapid thermal processing (RTP)

LAMMPS软件的简介

- LAMMPS: Large-scale Atomic/Molecular Massively Parallel Simulator
- 由美国能源部两个实验室发布(free and open-source)
- MD, MC → 从原子尺度到介观尺度
- CPU, GPU皆可，可并行
- 易于扩展，eg：添加力场方便
- 一个脚本可运行一个或多个模拟
- 非图形化界面
- 官网：http://lammps.sandia.gov/



LAMMPS输入文件

- 初试结构文件——data文件
- 模拟控制文件——in文件(input script)

1. Initialization
2. Atom definition
3. Settings
4. Run a simulation

- ✓ 每行命令中的不同字段由空格或者制表符分隔开来，每个字段可以由字母、数字、下划线、或标点符号构成；
- ✓ 每行命令中第一个字段表示命令名，之后的字段都是相关的参数；eg：units lj/real/metal/si/cgs　　units metal
- ✓ 注意：lammps里很多命令都有自己的默认设置，很多命令都是在需要修改默认值的情况下才特别设置的。

LAMMPS输入文件

- ✓ 每行后的“&”表示续行（类似fortran），“#”表示注释，$是跟声明变量有关的；
- ✓ 每一非空行都被认为是一条命令（大小写敏感，极少有命令或参数大写的）；
- ✓ 读入一行执行一行，有些命令在其他命令后有效，有些命令要用到其他命令的输出；比如，要设定一组原子的温度，需要先用group命令定义哪些原子属于这个组才行；
- ✓ in文件中各命令的顺序可能会对计算产生影响，但大部分情况下不会有影响；

LAMMPS输出文件

- log.lammps文件——记录了整个计算过程屏幕上显示的所有信息
- dump文件——输出应力、能量、原子位置、速度等，由dump命令控制输出文件，eg：xyz文件
- restart文件——断点续算文件，由write_restart命令控制。

data文件实例

```
# a-C@Ni

3 atoms
2 atom types

0 12.4592 xlo xhi
0 12.9480 ylo yhi
0 60.0000 zlo zhi

Masses

1 12.0107
2 58.6934

Atoms

   1  1 0.0     7.366430000   11.931600000   29.905000000
   2  2 0.0     0.202289000   12.728100000   11.926800000
   3  2 0.0    10.202289000   22.728100000   20.926800000
```

in文件实例

 # a-C@Ni

1. Initialization

units real #能量单位

newton on #turns Newton's 3rd law on or off for pairwise and bonded interactions

dimension 3 #模拟盒子的维度

boundary p p p #盒子三个反向都是三维周期的

2. Atom definition

atom_style charge #模拟中原子处理类型（带电荷的）

read_data data.Ni-C-600K-final #读取结果文件

pair_style reax/c lmp_control #用ReaxFF处理pairwise interaction

pair_coeff * * ffield.reax.FC C Ni #不同元素pairwise的力场参数

3. Settings

neighbor 2.0 bin #building of neighbor list 距离 算法

neigh_modify every 10 delay 0 check no #building and use of neighbor list

fix 1 all qeq/reax 1 0.0 10.0 1.0e-6 reax/c #Qeq方法处理电荷结合ReaxFF

in文件实例

4. Run a simulation with output (thermo & dump)

```
minimize 1.0e-12 1.0e-12 1000 1000
min_style cg
min_modify dmax 0.2

timestep 0.25
run_style verlet

fix 2 all nvt temp 900 900 1.0
thermo 40
thermo_style custom time temp press pe ke etotal enthalpy
dump 1 all xyz 40 a-C-on-Ni-900K.xyz
run 60000
unfix 2
undump 1
```

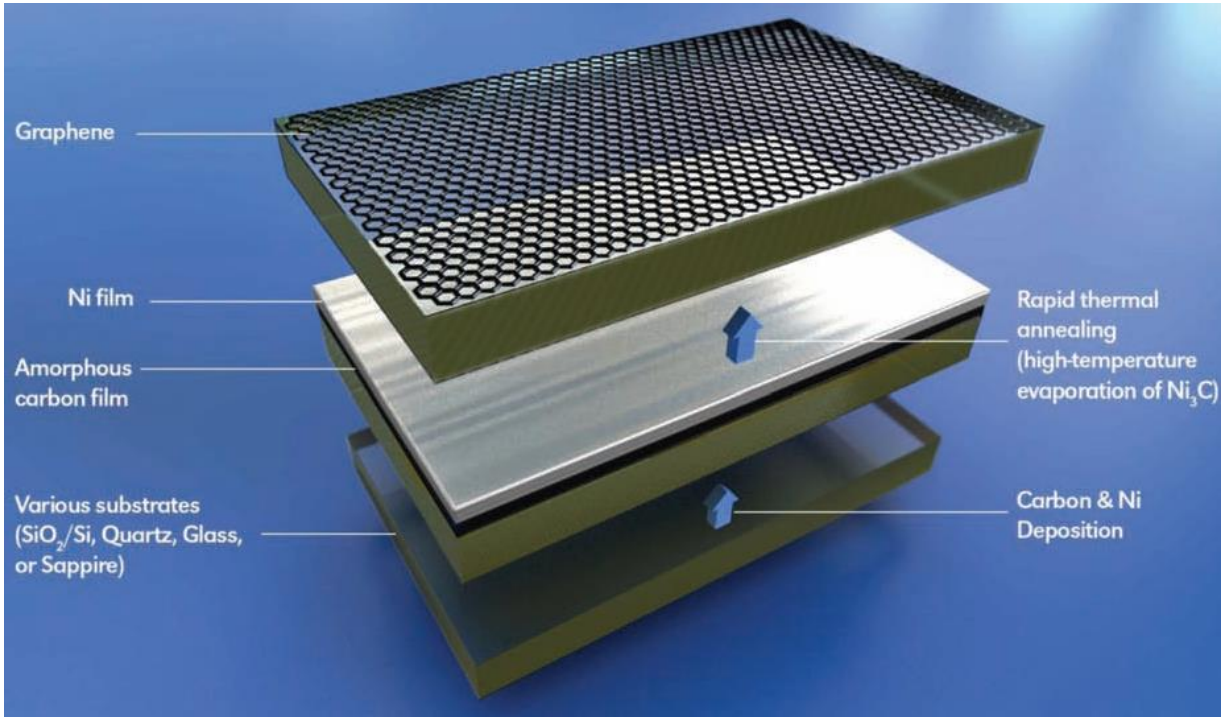
Geometry Optimization

MD

Ab Initio Molecular Dynamics Simulations of Nickel-Catalyzed Transformation of Amorphous Carbon into Graphene in Rapid Thermal Processing

Graphene Growth in Rapid Thermal Processing (RTP)

- Ni evaporation at 1100° C much lower than the Ni evaporation point



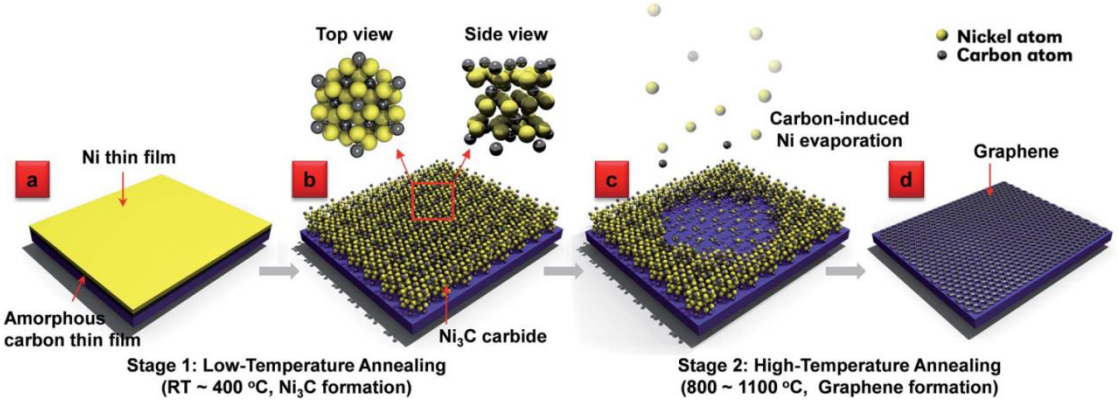
Compared to CVD:

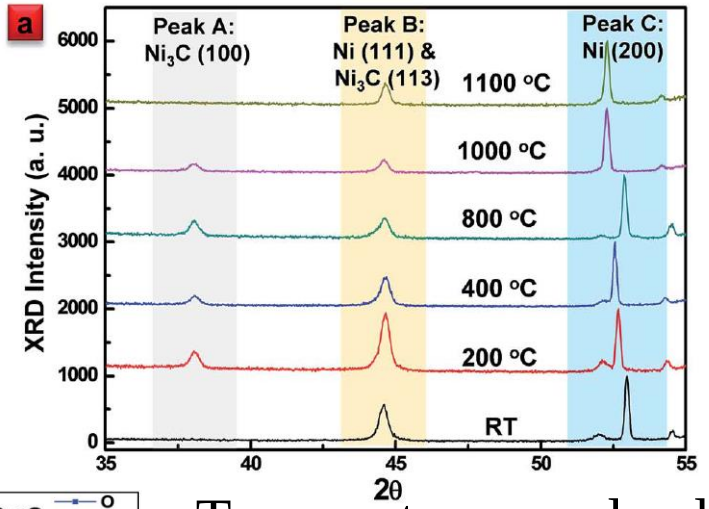
- No post-growth Ni etching
- Transfer-free (directly grown on various dielectric surfaces)
- Control number of graphene layers

Adv. Mater. **2013**, *25*, 630-634.

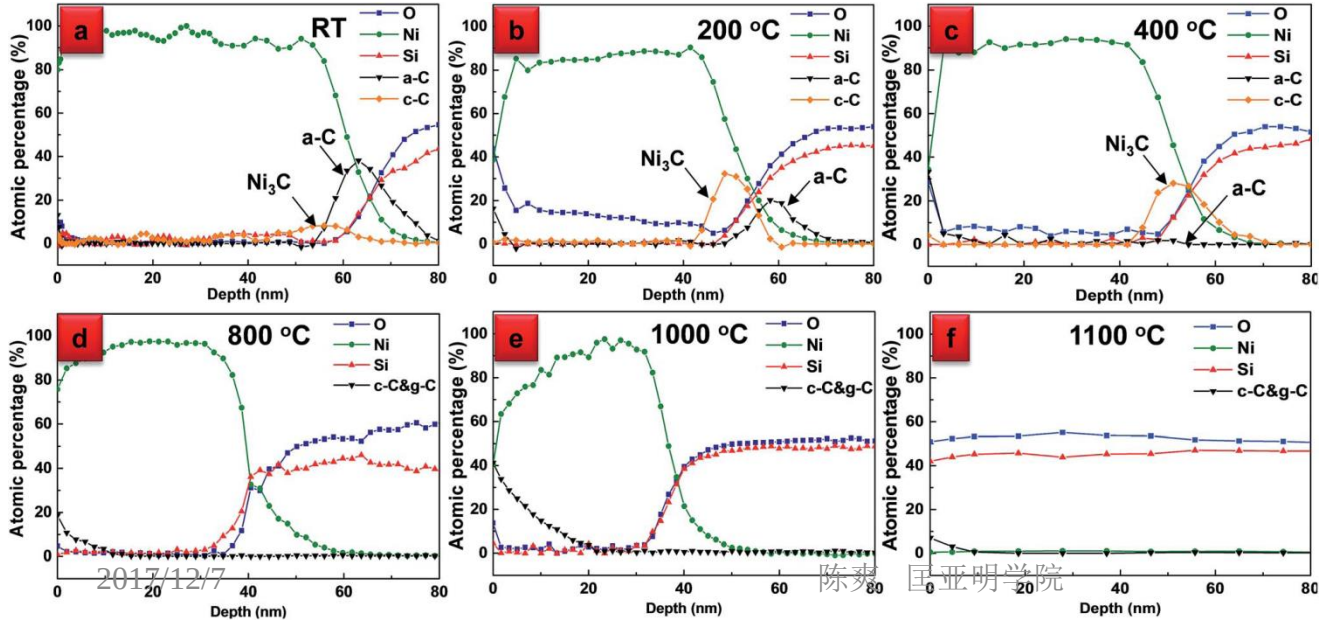
Graphene Growth in Rapid Thermal Processing (RTP)

- Formation of metastable Ni_3C





Temperature-resolved glancing-angle XRD

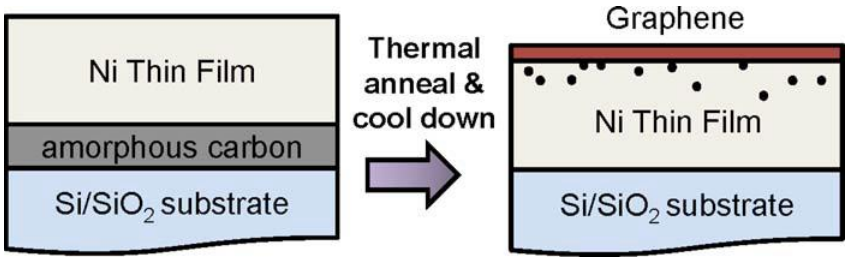


Temperature-resolved AES

RSC Adv. **2015**, *5*, 99037-99043.

Heating and Cooling of *a*-C/Ni Bilayer

- Ni-catalyzed *a*-C → graphene (top layer)



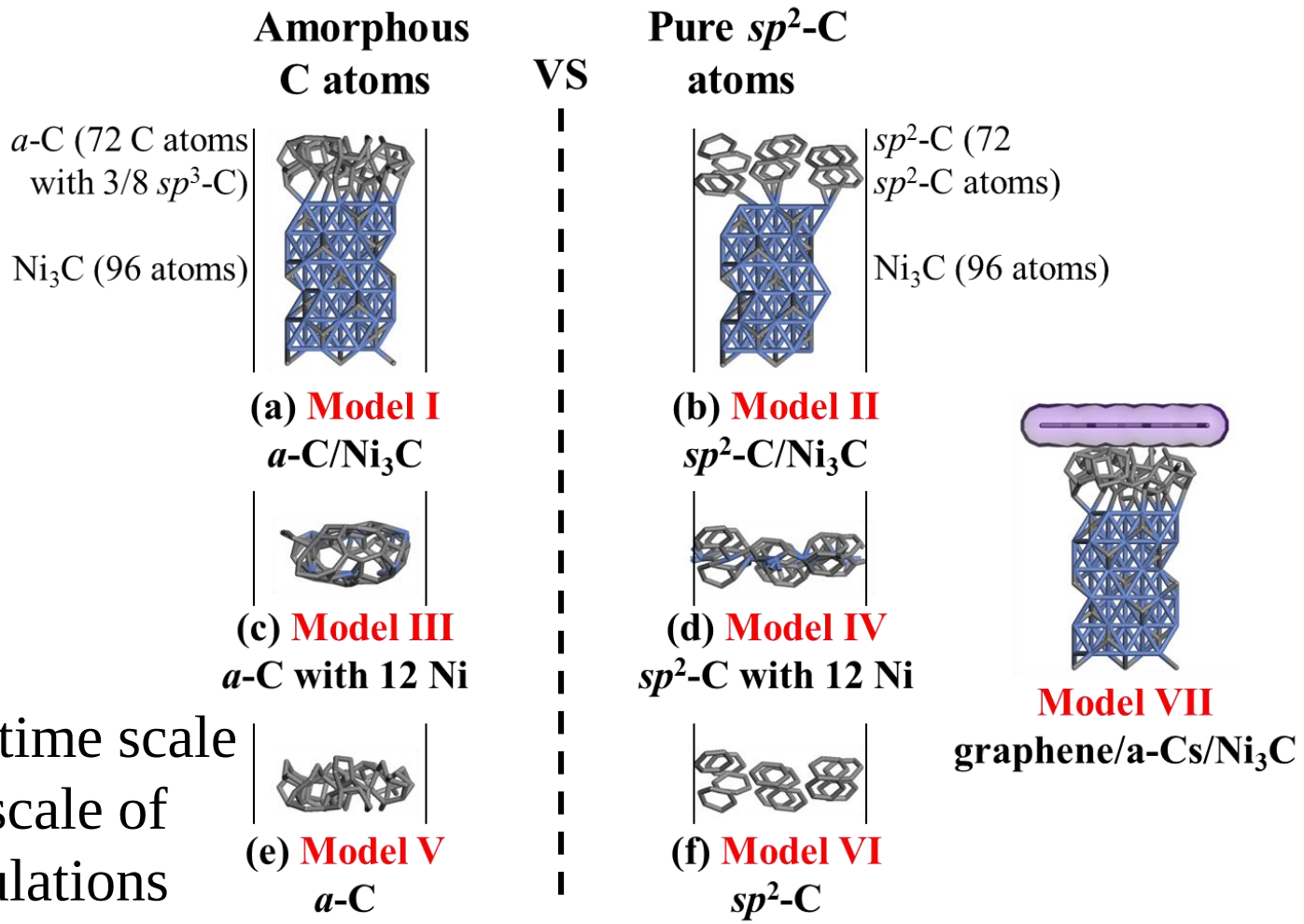
Appl. Phys. Lett. **2010**, *96*, 063110.

Appl. Phys. Lett. **2010**, *96*, 153105.

C in Ni:
- Low concentration
- High transport rate

- Graphitic C formation: 640−730° C
- Metal-induced crystallization and layer exchange mechanism (not a dissolution/precipitation mechanism)
- Reverse dissolution of graphitic C: > 950° C

Design of AIMD Slab Models



Limited by time scale and length scale of AIMD simulations

Chen, S. et al. *Nanoscale* **2016**, *8*, 9746-9755.

Computational Details

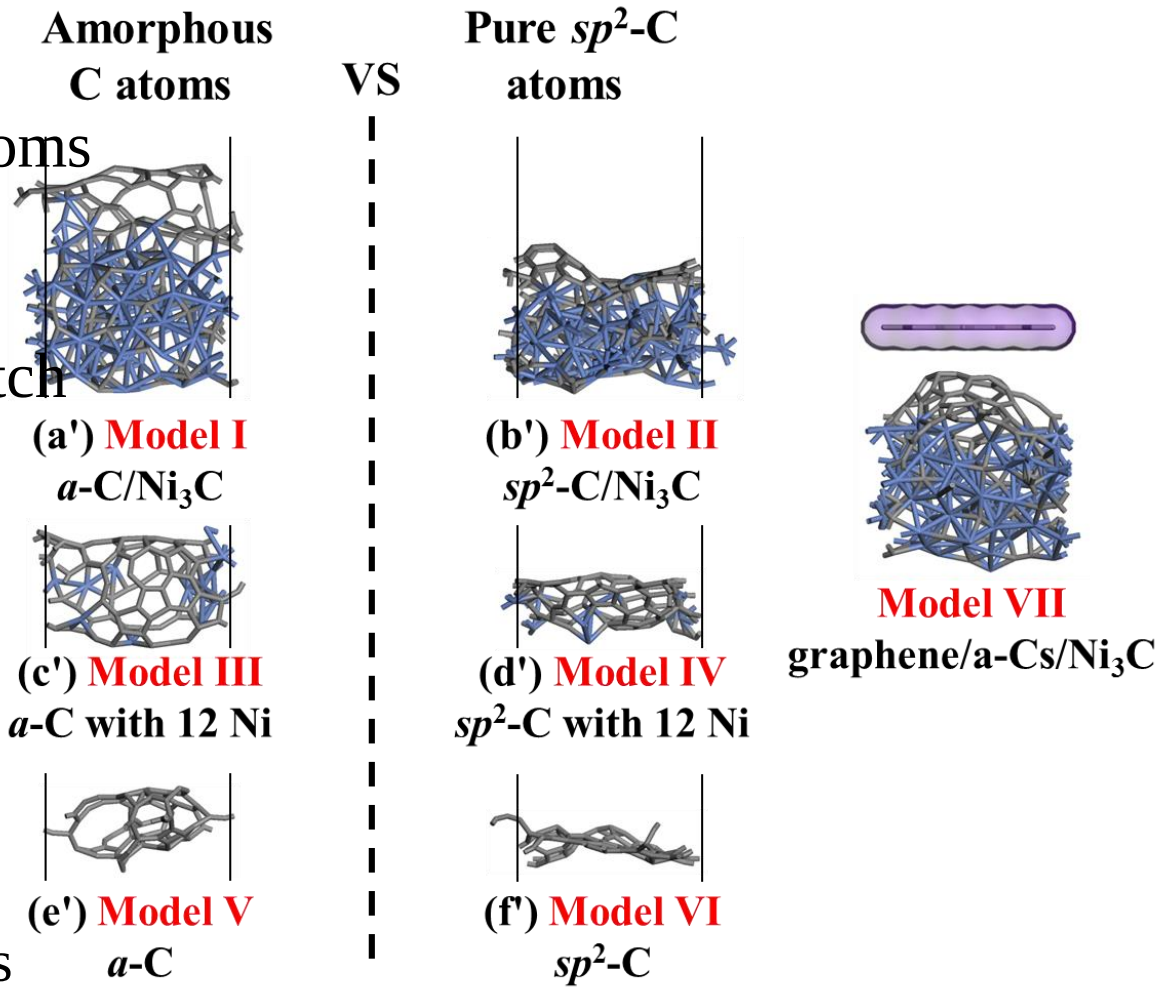
- Simulation setting (AIMD simulations in CP2K)

- *NVT* ensemble with **stepwise temperature (*T*) increasing: 300 K, 600 K, 900K, 1200 K, 1800 K,** (2400 K, and 3000 K)
- Each temperature with **15-ps** AIMD running
- PBE-D3 (dispersion cutoff radius: 20 Å)
- Gaussian plane-wave (GPW) method: GTH pseudopotential (330 Ry) + DZP (33 Ry)
- SCF: 10^{-6} a.u.
- Time step: 1 fs
- Nosé-Hoover chain thermostat

Chen, S. et al. *Nanoscale* **2016**, *8*, 9746-9755.

Final Snapshots (After 75 ps and 1800 K)

- Phase separation (C atoms can enter Ni_3C layer.)
- Localized dome-like patch vs relatively flat patch
- Carbon roll/shell vs flat patch
- Catalysis of Ni atoms
  - Stabilize the dangling C atoms
  - Support newly-formed graphene
- Formations of Ni clusters



Chen, S. et al. *Nanoscale* **2016**, *8*, 9746-9755.

模拟的实施

- Model building: amorphous C atoms@Ni(111) surface by MS → generate data file
- Step-by-step temperature increasing simulations with *NVT* ensemble: 300 K →…→ 3000 K
- Put data, in, ffield.reax.FC, and lmp_control files into E:\Program Files\LAMMPS 64-bit 20170127\bin
- 运行cmd
- 往下输入命令：

✓ E:

✓ cd E:\Program Files\LAMMPS 64-bit 20170127\bin

✓ set OMP_NUM_THREADS=2

✓ lmp_mpi.exe < in file name

- xyz轨迹文件可用VMD软件读取