Crystal Structure Prediction via Particle Swarm Optimization (PSO): Theory and applications

Ma Yanming
State Key Laboratory of Superhard Materials
Changchun
P.R. China
Crystal Structure Prediction via Particle Swarm Optimization (PSO): Theory and applications

Yanming Ma

In collaboration with Y. Wang, J. Lv, and L. Zhu

State Key Lab of Superhard Materials, Jilin University

2011.1.14
Outline

1. Introduction
2. Principles of Particle Swarm Optimization
3. Benchmark and Applications
4. Conclusions and Perspectives
Structure is the basis for understanding materials and their physical properties

- Electric property
- Optical property
- Mechanical property
- Thermal property
- Magnetism

Crystal structure is the basis for understanding materials and their physical properties.
Experimental methods for structural determination

Experiments:
- X-ray diffraction
- Neutron scattering
- X-ray diffraction and high resolution SEM

Difficulties:
- Impurity of the sample
- Poor diffraction data
- Extreme external conditions (e.g., high pressure)

Crystal structure prediction is essential
What is the challenge of crystal structure prediction?

Finding the GLOBAL stable structure (i.e., energy minimum) on the complex energy landscape with only given chemical compositions

Trying all possible structures is impossible !!!!

<table>
<thead>
<tr>
<th>$N_{\text{atoms}}$</th>
<th>Structural Variants</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>$10^{25}$</td>
</tr>
<tr>
<td>30</td>
<td>$10^{39}$</td>
</tr>
</tbody>
</table>

$$C = \frac{1}{(V/\delta^3) \left[ (V/\delta^3) - N \right]! N!} \frac{(V/\delta^3)!}{(V/\delta^3)!}$$
Earlier Methods and Principles

1. Use of available structure database
   - Data Mining [Christopher, Nat. Mater. 5, 641 (2006)]
   - Substitutional Method [Mujica, PRB 55, 9659 (1997)]

2. Random sampling approach
   - C. Pickard and R. Needs [PRL 97, 045504 (2006)]

“simple” in principle but nontrivial in practice
3. Energy barrier Hopping

- Metadynamics [Martonak, PRL 90, 75503 (2003) ]
- Basin Hopping  [Wales, JPCA 101, 5111 (1997) ]
- Minima Hopping [Goedecker, JCP 120,9911 (2004) ]

Conquering the energy barrier

4. Genetic algorithm (GA)

- Deaven , PRL 75, 288 (1995)
- USPEX [Oganov, JCP 124, 244704 (2006) ]
- GSGO [Zunger , PRB 75, 104113, 2007]

Operation: cross over and mutation
Advantage: self-improving via evolution
Particle Swarm Optimization (PSO)

Kennedy and Eberhart 1995

- Swarm search
- Information exchanges between Individual particles
- Self-improving evolution
- Swarm Intelligence
- Particles evolve by tracing with the optimal Particle
Principle of PSO
Application of PSO on crystal structure prediction

Parallel algorithm

Crystal structure prediction

Artificial Intelligence

Neural network

Power Distribution

Computer network Distribution

PSO
PSO Principle on structural prediction

Particle
✓ Position
✓ Velocity
✓ Fitness

\[ x_{i,j}^{t+1} = x_{i,j}^t + v_{i,j}^{t+1} \]

\[ v_{i,j}^{t+1} = \omega v_{i,j}^t + c_1 r_1 (p\text{best}_{i,j}^t - x_{i,j}^t) + c_2 r_2 (g\text{best}_{i,j}^t - x_{i,j}^t) \]
CALYPSO code

Crystal structure AnaLYsis by Particle Swarm Optimization

CALYPSO

➢ The name of the Nereids (sea nymphs) in Greek mythology
➢ A genre of Trinidadian folk music

Input parameters: chemical compositions and external conditions (e.g. high pressure)

China copyright protection via No.2010SR028200
Features of CALYPSO

1. Randomly generated structures (symmetrical constraint)
   - Reduction of the search space
   - Increase of structural diversity to avoid trapping into local minimum

2. Locally Structural Optimization
   - Reduction of the noise of the energy landscape

3. Geometrical Structure Parameter (Similar function)
   - Elimination of duplicated structure and determination of non-fly area to improve search efficiency

4. Particle Swarm Optimization (Swarm Intelligence and self-improving)
   - Swarm Intelligence through information exchanges
   - Control of particle speed and direction by optimal particle to accelerate convergence
   - Excluding unfavorable energy landscape through self-improving to reduce the search space
Outline

1. Introduction
2. Principles of Particle Swarm Optimization
3. Benchmark and Applications
4. Conclusions and Perspectives
## Benchmark of CALYPSO

<table>
<thead>
<tr>
<th>System</th>
<th>Pressure (GPa)</th>
<th>Structure</th>
<th>Generation</th>
<th>Population size</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li</td>
<td>0</td>
<td>Bcc</td>
<td>1</td>
<td>30</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>9R</td>
<td>3</td>
<td>30</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>Fcc</td>
<td>1</td>
<td>20</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>hR1</td>
<td>4</td>
<td>30</td>
</tr>
<tr>
<td></td>
<td>70</td>
<td>cI16</td>
<td>7</td>
<td>30</td>
</tr>
<tr>
<td>C</td>
<td>0</td>
<td>Graphite</td>
<td>30</td>
<td>30</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>Diamond</td>
<td>6</td>
<td>30</td>
</tr>
<tr>
<td>Si</td>
<td>2</td>
<td>Bc8</td>
<td>6</td>
<td>30</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>cd</td>
<td>1</td>
<td>20</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>sh</td>
<td>2</td>
<td>20</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>β-Sn</td>
<td>3</td>
<td>20</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>Imma</td>
<td>4</td>
<td>20</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>Cmca</td>
<td>2</td>
<td>20</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>Hcp</td>
<td>4</td>
<td>20</td>
</tr>
<tr>
<td></td>
<td>80</td>
<td>Fcc</td>
<td>1</td>
<td>20</td>
</tr>
<tr>
<td>Mg</td>
<td>0</td>
<td>Hcp</td>
<td>6</td>
<td>30</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>Bcc</td>
<td>4</td>
<td>30</td>
</tr>
</tbody>
</table>
## Benchmark of CALYPSO

<table>
<thead>
<tr>
<th>System</th>
<th>Pressure (GPa)</th>
<th>Structure</th>
<th>Generation</th>
<th>Population size</th>
</tr>
</thead>
<tbody>
<tr>
<td>SiO₂</td>
<td>0</td>
<td>α-quartz</td>
<td>5</td>
<td>20</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>Stishovite</td>
<td>1</td>
<td>20</td>
</tr>
<tr>
<td></td>
<td>70</td>
<td>CaCl₂-type</td>
<td>5</td>
<td>30</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>α-PbO₂-type</td>
<td>4</td>
<td>20</td>
</tr>
<tr>
<td></td>
<td>500</td>
<td>Pyrite-type</td>
<td>15</td>
<td>20</td>
</tr>
<tr>
<td>SiC</td>
<td>0</td>
<td>Zinc blende</td>
<td>6</td>
<td>30</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>Moissanite</td>
<td>3</td>
<td>30</td>
</tr>
<tr>
<td></td>
<td>150</td>
<td>Rock salt</td>
<td>2</td>
<td>30</td>
</tr>
<tr>
<td>ZnO</td>
<td>12</td>
<td>Rock salt</td>
<td>2</td>
<td>30</td>
</tr>
<tr>
<td>TiH₂</td>
<td>0</td>
<td>I4/mmm</td>
<td>2</td>
<td>20</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>Fm-3m</td>
<td>3</td>
<td>20</td>
</tr>
<tr>
<td>MoB₂</td>
<td>0</td>
<td>R-3m</td>
<td>1</td>
<td>30</td>
</tr>
<tr>
<td>TiB₂</td>
<td>0</td>
<td>AlB₂-type</td>
<td>1</td>
<td>30</td>
</tr>
<tr>
<td>MgSiO₃</td>
<td>120</td>
<td>Cmcm</td>
<td>5</td>
<td>20</td>
</tr>
<tr>
<td>CaCO₃</td>
<td>0</td>
<td>Calcite</td>
<td>13</td>
<td>30</td>
</tr>
</tbody>
</table>
Benchmark of CALYPSO

CaCl$_2$ structure

Calcite structure

SiO$_2$ at 70GPa

CaCO$_3$ at 0GPa

## Comparison with GA

<table>
<thead>
<tr>
<th>Systems</th>
<th>Algorithm</th>
<th>Pressure (GPa)</th>
<th>Structures</th>
<th>Generations</th>
<th>N\textsubscript{pop}</th>
<th>N\textsubscript{opt}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>PSO</td>
<td>0</td>
<td>Diamond</td>
<td>8/5</td>
<td>16</td>
<td>128/5</td>
</tr>
<tr>
<td></td>
<td>GA\textsuperscript{a}</td>
<td>0</td>
<td>Diamond</td>
<td>15</td>
<td>16</td>
<td>60</td>
</tr>
<tr>
<td>SiC</td>
<td>PSO</td>
<td>0</td>
<td>Zinc blende</td>
<td>8/5</td>
<td>12</td>
<td>96/5</td>
</tr>
<tr>
<td></td>
<td>GA\textsuperscript{a}</td>
<td>0</td>
<td>Zinc blende</td>
<td>5</td>
<td>12</td>
<td>20</td>
</tr>
<tr>
<td>GaAs</td>
<td>PSO</td>
<td>0</td>
<td>Zinc blende</td>
<td>16/5</td>
<td>12</td>
<td>192/5</td>
</tr>
<tr>
<td></td>
<td>GA\textsuperscript{a}</td>
<td>0</td>
<td>Zinc blende</td>
<td>19</td>
<td>12</td>
<td>70</td>
</tr>
</tbody>
</table>

GA data taken from Trimarchi and Zunger, PRB 75, 104113 (2007)
Carbon polymorphs by CALYPSO

a. BC₈
b. C₆

c. β-Sn
d. P6₅22

Metastable phases of Carbon
Metal-insulator transitions in Lithium and Sodium under pressure

High pressure insulating structures of Li

Direct observation of a pressure-induced metal-to-semiconductor transition in lithium

Takahiro Matsuoka & Katsuya Shimizu

![Graph showing resistivity and pressure loading](image)

![Graph showing resistance change with temperature](image)
Prediction of the most favorable insulating structure of Li

Li at 80 GPa (Aba2-40)

Lv, Wang, Zhu, and Ma, PRL 106,015503 (2011)
Li at 80 GPa (orthor.)
Experimental confirmation?

Cold melting and solid structures of dense lithium, Guillaume et al, Nature physics, DOI: 10.1038/NPHYS1864, (2011)
Outline

1. Introduction
2. Principles of Particle Swarm Optimization
3. Benchmark and Applications
4. Conclusions and Perspectives
Conclusions

PSO on crystal structure prediction

1. **Wide range of applications**
   Metals, semiconductors, insulators and ionic crystals, etc.

2. **Fast convergence**
   Number of local optimization < 300

3. **High success rate**
   The success rate of prediction on elemental, binary and ternary compounds is nearly ~100%

4. **Capable on Prediction of meta-stable structures**
Welcome to use CALYPSO package

Webpage: http://nlshm-lab.jlu.edu.cn/~calypso.html

Please send to YM (mym@jlu.edu.cn) for request
Thanks !!!