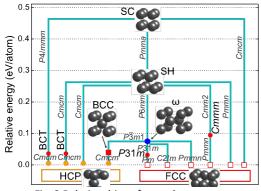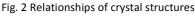# Software development for transition pathway search in crystals

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Abstract: We have been making software developments for crystal symmetry finder (spglib[1]) and phonon code (phonopy[2]). Spglib can find space-group type and its operations from basis vectors and points of atoms in a unit cell. Phonopy needs forces on atoms or force constants as inputs from first-principles calculations to obtain useful phonon properties, e.g., free energy, thermal displacements, thermal expansion, and lattice thermal conductivity. Spglib and phonopy are designed to be used as parts of other software. Spglib is written as a C-library and phonopy can be used as a Python module. We applied these for an automated transition pathway search in crystals[3]. The basic idea is just simple. Starting with a high-symmetry but dynamically unstable crystal structure, it is systematically relaxed following phonon eigenvectors that show dynamical instabilities. Once a calculation starts, a tree-like shaped transition pathway is obtained automatically as shown in Fig. 1. Continuous relationships of crystal structures are recorded and the space-group types of crystal structures and transition pathways are simultaneously assigned as shown in Figs. 1 and 2. This research is appropriate to let computers do since it requires a lot of effort if we make it by hand. I plan to talk about overview of these software and the algorithms. I may also talk about our recent research on phonon-phonon interaction[4].
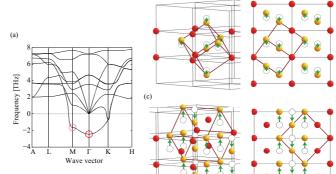
Fig. 2 Relationships of crystal structures

Fig.1 Transition pathway of Cu. (a) Phonon band structure of ω-phase, and (b) ω to BCC and (c) ω to FCC pathways.

[1] http://spglib.sourceforge.net/
[2] http://phonopy.sourceforge.net/
[3] A. Togo and I. Tanaka, Phys. Rev. B, b, 184104 (2013)
[4] A. Togo, L. Chaput, and I. Tanaka, Phys. Rev. B 91, 094306 (2015)