A comprehensive platform to simulate TEM images and materials properties by first principles method; An introduction to MedeA

Atsushi Fujiwara, Kouji Chiba

Science and Technology System Division, Ryoka Systems Inc., Tokyo, 104-0033, Japan

Recently, atomistic simulation is used in a wide variety of fields, even in industrial researches and developments, as well as in academic studies. This prevalence is encouraged by the rapid progress in hardware technologies known as high performance computing, which brings us a powerful environment for simulation on realistic (rather big) size of systems in reasonable time. At the same time, software development has also been advanced with hardware progress. Under the condition of such concerted progress, not only technical advancements for speed up of calculations or new scientific methods but also improvements in working environments such as graphical user interface (GUI) are becoming important more and more. GUI supplies intuitive and efficient environment so that users can work with first principles calculation simply, rightly and quickly. Its user-friendliness helps many beginners to be familiar with simulation. As a result, nowadays, first principles calculation has been becoming a common tool to investigate material properties.

MedeA is a software package developed by Materials Design [1], a company in USA. It supplies a comprehensive platform to investigate various material properties by enabling us to build model structures, run calculations and analyze results on GUI environment (Fig. 1). Practical tools implemented in MedeA enable users to evaluate further advanced and industrial properties like lattice vibration and mechanical properties based on first principles calculation automatically, as well as basic physical values such as electronic energy and stable structures which are available from usual first principles calculation. In addition, convenient modeling tools are also developed, for instance, “Interface Builder” can build twist grain boundaries and interfaces by searching optimal matches between two interfaces of exhaustive geometric matches. Successful applications using MedeA are reported even in industrial researches [2].

Furthermore, recently a tool named JEMS [3] for the calculation of TEM images and related structure analysis (Fig. 2) is implemented in MedeA. It supports not only the Bloch wave method but also the multislice method based on the dynamical theory of electron diffraction. The combination of MedeA and JEMS conduce a powerful and efficient environment for analysis of lattice structure.

References

[1] Materials Design; http://www.materialsdesign.com/
[2] E. Wimmer et al., J. Phys. Condens. Matter 22 (2010) 384215.
[3] JEMS is developed by Prof. Pierre A. Stadelman from Centre Interdepartmental de Microscopie Electronique, Ecole Polytechnique Fédérale de Lausanne in Switzerland; see also http://cimewww.epfl.ch/people/stadelmann/jemswebsite/jems.html.

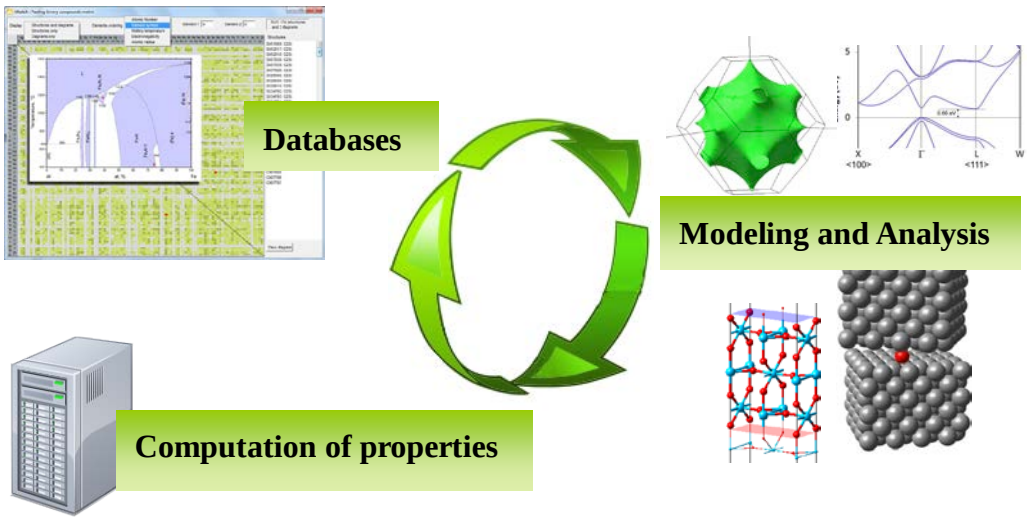

FIG. 1. The comprehensive platform of MedeA. MedeA has databases of experimental and computed structures and properties, which supply a base of system to start a calculation. By using a structure from databases, we can work on modeling such as inserting impurities, generating defects, constructing a surface slab model and grain boundary, etc. with GUI on MedeA. Calculation on the constructed models can be submitted to servers just by clicking a mouse button, and then the results are collected and stored in a database automatically. The result stored in databases can be used for analysis and subsequent calculations.

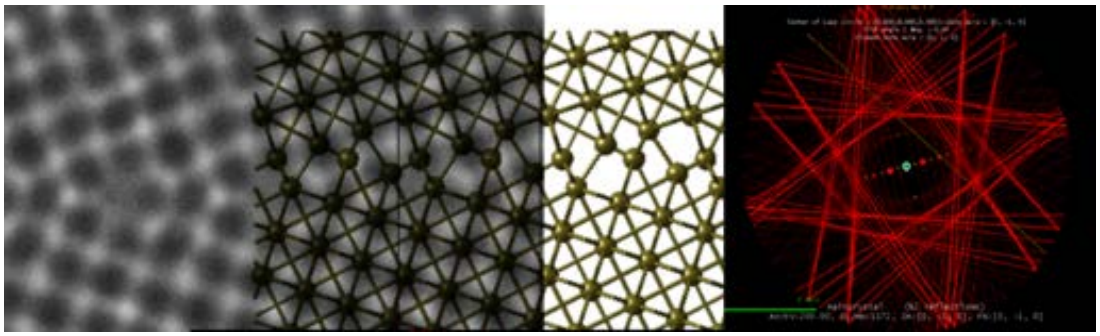

FIG. 2. MedeA-JEMS. A simulated HRTEM image of a Σ5(310) grain boundary in Au (left), the structure generated by MedeA's Interface builder, as well as the diffraction pattern (right) of the shown structure (center).