First-principles study of energetics of slip deformation in NaCl and AgCl

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Alkali halide crystals having the sodium chloride structure are generally brittle at low temperatures, and thus were often used as models to study a fundamental fracture mechanism in brittle materials such as ceramics. The brittle mechanical properties are closely related to primary slip systems that determine dislocation glides in the crystals. For instance, an {110}<110> system is only activated in NaCl crystals and other slip systems are not ordinarily activated, resulting in the easy cleavage fracture due to the limited slip system. In contrast, AgCl having the same sodium chloride structure is more ductile than NaCl. In fact, it was reported that slip systems along {100} and {111} can be activated in AgCl, in addition to the slip system along {110} [1]. However, little is known about the difference in primary slip systems between NaCl and AgCl. In order to address this issue, first-principles calculations were performed to analyze energetics of slip deformation in NaCl and AgCl, and a physical origin of the different slip systems in these crystals was discussed.

In this study, the projector augmented wave (PAW) method in the Vienna Ab-initio Simulation Package (VASP) was used [2]. The generalized gradient approximation (GGA) was selected for the exchange correlation potential [3]. As an initial structure, slab models of perfect crystals were constructed, and supercells with the slabs sandwiched by vacuum were used. For calculations of slip deformation, a half crystal in a slab model was rigidly and gradually displaced along a particular slip plane and direction, and atomic structures were then optimized with keeping the displacement. Total energy variations against displacements were analyzed to investigate whether the slip system can be activated or not, in comparison with surface energies. Structure optimizations were performed until residual forces on atoms were less than 0.01 eV/Å. Energy profiles against displacement thus obtained correspond to generalized staking fault (GSF) energies, which were used to theoretically estimate Peierls stresses by Joós et al. [4]

Figure 1 shows GSF energies in NaCl and AgCl along the <110> slip direction on several slip planes. As can be seen in (a), GSF energies along {100} and {111} were larger than the double of the {100} surface energy, $2\gamma_s$. This indicates that activation of these slip systems can bring about cleavage fracture. In the case of {110}, the GSF energy was lower than $2\gamma_s$ for {100} and {110}, which indicates only the {110}<110>

slip system can be activated in NaCl. In contrast, the GSF energies along {110}, {100} and {111} in AgCl were lower than $2\gamma_s$ of {100} and {110}. Moreover, the values of GSF energies were lower, even compared to the case of NaCl. It can be said, therefore, that the several primary slip systems can be activated in AgCl, unlike the case in NaCl.

Acknowledgement
The authors gratefully acknowledge the financial support by a Grant-in-Aid for Challenging Exploratory Research from Japan Society for the Promotion of Science (JSPS).

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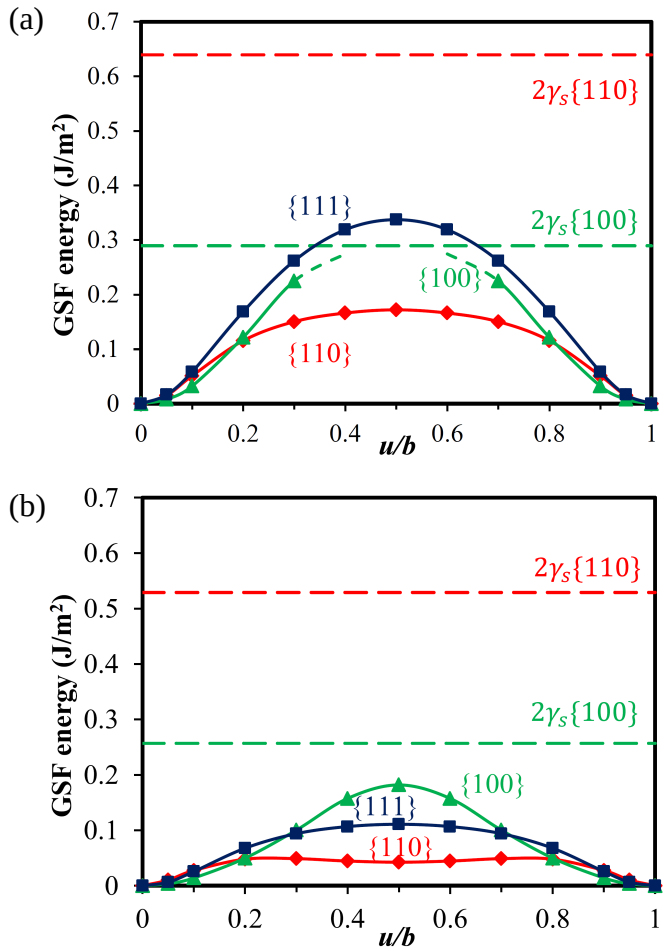

Fig.1. GSF energy curves for (a) NaCl and (b) AgCl, as a function of the displacement *u* divided by the Burgers vector. These results are for the slip direction of <110>.