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First-principles study on the electromigration of oxygen vacancy in metal oxides SANG HO JEON, WON-JOON SON, BAE HO PARK, SEUNGWU HAN, DEPARTMENT OF PHYSICS, KONKUK UNIVERSITY TEAM, DEPARTMENT OF PHYSICS, EWHA WOMANS UNIVERSITY TEAM — The oxygen vacancy, which is a fundamental defect in oxides, plays a critical role in defining many electrical properties of oxides ranging from ionic conductivities to leakage behaviors. As such, to control the density and spatial distribution of the oxygen vacancy has often been an important goal in many researches on electronic devices, particularly for high-density devices, such as resistance-change random access memories(ReRAM). Despite its importance, the electromigration of oxygen vacancy has not been studied much from the microscopic point of view. In this presentation, we studied on the migration of the oxygen vacancy in metal oxides, such as MgO and TiO2. First, using the nudged elastic band(NEB) method, we estimated the migration barrier of charged oxygen vacancy under an external field. Then, we calculate the zone-center phonon modes of the bulk system to obtain the attempt frequency of the vacancy diffusion. Based on these results, we estimated the migration time of oxygen vacancy in metal oxide by using harmonic transition state theory, and it was in good agreement with the result of molecular dynamics(MD) calculation.

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