「赤外光励起による半導体中の不純物拡散の制御」

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Control of impurity diffusion by IR excitation

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Control of impurity diffusion is an important element in the device technologies of the present days. Usual thermal processes have an inherent disadvantage that not only the intended species but also all impurities involved are equally affected. This imposes many restrictions on the device process. In order to remove such restrictions, it is desirable to diffuse the specific species only. One of such attempts is use of infrared (IR) excitation [1]. The idea is that every impurity has its own local vibrations in the host crystal. The frequency is dependent of impurity species. Irradiation of IR laser with the resonant frequency could cause excitation of the local impurity modes, which results in the selective enhancement of the diffusion of that impurity. Unfortunately, there is a well-known and big problem for this aim, that is, there is no suitable IR laser source. In hoping that this technical problem will be solved in near future, we have performed first-principles (FP) molecular dynamics (MD) simulations.

The missions of the theoretical study are to confirm this effect by simulations, and, if effective, to derive the conditions where this effect appears. This makes it possible to design the laser experiment, if appropriate light sources are available. The phenomena which are encompassed in this simulation are indeed in a wide range, from identification of impurity modes, IR resonance effects, finally to diffusion phenomena. Therefore, this kind of simulation itself is a challenge for the MD simulation based on the density-functional theoretic method [2-3]. We observe that IR excitation is effective for O and B impurities, while is ineffective for P. In case of P, the impurity mode is buried in the host phonon band, so that resonance effect is not appreciable.

Based on the present simulations, we are able to design the IR excitation experiment in order to observe an appropriate effect on atom migrations. The needed power of IR laser depends on the lifetime of the local mode under investigation. The lifetime of phonons is basically predictable by *ab initio* calculations [5, 6]. For those modes of sufficient long lifetime, a design of a real experiment is given in this study. Based on these FP-MD simulations, we have drawn the first draft of experiment in SPring-8 facility.

References: [1] H. Yamada-Kaneta and K. Tanahashi, Physica B **376-377**, 66 (2006). [2] K. Shirai and H. Katayama-Yoshida, *Proc. 4th Int. Symp. on Advanced Sci. and Tech. of Silicon Materials*, 2004, Hawaii, p129. [3] K. Shirai, *et al.*, J. Phys.: Condensed Matters, *in press*. [4] K. Shirai, et al., Physica B **376-377**, 41 (2006). [5] K. Shirai and H. Katayama-Yoshida, Phys. Soc. Jpn. **67**, 3801 (1998).