

## Formation of compensating defects through many-body interaction

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### Abstract

Recently the high conductive and high speed transparent conducting oxides (TCO) is demanded for the high-speed and high-density transparent touch screen display. In spite of great efforts, the maximum carrier concentration in the TCO is limited around  $2 \times 10^{21} \text{ cm}^{-3}$ , for which the compensating defects or some clustering were indicated to play roles. However, the microscopic understanding of the doping limit of TCO and the defect formation are not yet clearly resolved.

In the extremely heavily doped semiconductors, a defect becomes to interact with many dopants, which can change the formation energy of the defect. In this work, it is found that the doping limit can be induced by the interaction between the compensating defect and the dopants, which comes from the Coulomb interaction. It is found that as the concentration of dopant becomes higher than about  $10^{21} \text{ cm}^{-3}$ , the effect of interaction becomes emerging, and the high concentration of compensating defect, comparable to the dopant concentration, are generated, which leads to the doping limit. We discuss the more detail of the conventional theory of the heavily doped semiconductors according conventional theory based on the formation enthalpy.

**Keywords:** Semiconductor, doping, defect