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Intrinsic point defects and their interaction with impurities in mono-crystalline zinc oxide

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Zinc oxide (ZnO) is a direct and wide band-gap semiconductor with several attractive features, like an exciton binding energy of $\sim$ 60 meV, for light emitting devices, photovoltaics and spintronics. In the past decade, ZnO has received tremendous attention by the semiconductor physics community and many challenging issues have been addressed, especially the "native" n-type conductivity, the role of intrinsic point defects, and the realization of reproducible p-type doping. The latter is, indeed, decisive for a true breakthrough of ZnO-based optoelectronics. In this contribution, recent progress in our understanding of the interaction between intrinsic point defects and impurities in ZnO will be discussed. Aluminum (Al) is often introduced intentionally to accomplish high n-type conductivity since Al on Zn-site (Al_{Zn}) acts as a shallow donor. However, Al_{Zn} was recently found to react strongly with Zn vacancies (V_{Zn}) and the resulting complex (Al_{Zn}-V_{Zn}) is energetically favorable. The Al_{Zn}-V_{Zn} complex is a deep acceptor limiting the n-type doping efficiency and this finding is expected to hold in general for complexes between V_{Zn} and group-III elements. Further, implantation of self-ions (Zn and O) has been demonstrated to affect radically the balance of intrinsic point defects where an excess of Zn interstitials gives rise to a dramatic depletion of residual Li impurities on Zn-site (Li_{Zn}) whilst the opposite holds for an excess of O interstitials. In fact, this behavior appears to be of general validity and Li depletion occurs for a wide variety of implanted elements incorporated into the Zn sub-lattice while Li pile-up occurs for elements residing on O-site. Finally, the most prominent deep-level defect in ZnO, labelled E3, will be shown to involve hydrogen. E3 exists in most ZnO materials, irrespective of the growth method used, and evidence for a center formed by reaction between interstitial hydrogen and primary defects on the Zn sub-lattice will be given.