Contribution ID: **107** Type: **POSTER**

The EFG at sp-impurities in Zn and Cd - a new (final?) look

The measurement of the nuclear quadrupole interaction at impurities in simple metals with nuclear methods, the PAC and PAD techniques in particular, has produced a great number of precise experimental data. For the 4sp and 5sp impurities in the strongly deformed hexagonal metals Zn and Cd the data set is almost complete. It has allowed to develop a qualitative understanding of the trends observed. Within a rigid band model [1] the sign change at group V impurities could be explained. Several early theoretical calculations with different methods have confirmed the conclusions but failed to reach quantitative agreement with the experimental data. The local lattice relaxation around the impurities has generally been blamed for this problem. The present work has been started to include this effect by the use of very large (150 atoms) supercells and the precise FLAPW method. For the cases where the nuclear quadrupole moments (Q) are reliably known the calculations reproduce quantitatively the data, with two exceptions: Ag in Zn and I in Zn and Cd. In the first case a generally not very reliable nuclear orientation measurement has been the data source [2]. For the second case the pioneering □-□ PAC experiment [3], however, appears quite reliable. A remeasurement with a different technique would be worthwhile. Whenever Q has only been estimated, strong disagreement is found. In these three cases (67Ge, 77Br, 123Xe) it is felt that the present work results in the first reliable value for Q. The qualitative features found can be understood in the rigid band model. An extensive estimation of the theoretical errors has been made using calculations with a 64 atoms supercell.

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Oral

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Track Classification: Theory: Hyperfine Interactions, Nuclear Moments