Configurational Defect Bistability in Semiconductors: The MFe Center in InP

*by G. A. Samara**

Motivation—One of the more interesting and important developments in the study of lattice defects and their associated deep electronic levels in covalent semiconductors has been the discovery that an ever-increasing number of important defects exhibit configurtional bistability (or multistability). Configurationally bistable defects are defects which, for the same charge state, can exist in two different configurations with distinct electronic and optical properties. Reversible transformations between the two configurations can be induced by thermal, electrical or optical means, and the configuration, which is observed experimentally, is dependent on the thermal, electronic and optical history of the sample. The MFe-center in Fe-doped n-InP is such a configurationally bistable defect. Although its properties have been characterized at 1 bar in considerable detail, much remains to be learned about the atomic structure of its two configurations and the nature of the transformations between them. In the present work we show that measurements under pressure shed much new light on the physics of this center.

Accomplishment—The MFe center, which is formed during high temperature p^+ doping (Zn^{2+} or Cd^{2+}) to form p^+/n junctions on Fe-doped InP, was first studied by Levinson, et al., (J. Electron Mats. 14a, 1133, 1985). When occupied by electrons, it can be reversibly placed in either of two configurations, A or B. A is obtained by cooling the junction with no applied bias, i.e., in the presence of electrons, whereas B is obtained by cooling under reverse bias, i.e., in the absence of electrons, followed by zero biasing to fill the traps. The signatures of the two configurations in thermally-scanned capacitance (TSCAP) and deep level transient spectroscopy (DLTS) are shown in Figs. 1 and 2. The emission from B has two steps, B1 and B2, each involving the emission of one electron. We find that hydrostatic pressure has drastic influence on the energetics and kinetics of the various processes associated with the MFe center. The energies and their pressure dependences as well as the activation volumes (ΔV^*) for these processes were determined. In the absence of barriers to electron capture, or for small barriers, ΔV^* can be interpreted as the breathing mode relaxation associated with electron emission or capture. At ≥ 8 kbar only the A configuration exists (Figs. 1 and 2) regardless of bias conditions during cooling because at these pressures the B$\rightarrow$A transition energy becomes the smallest energy of the problem (Fig. 3). These pressure results have allowed us to critically test a proposed atomic model for the MFe center. In this model the A configuration is taken to be the Fe anti-site/In vacancy complex, $Fe_{In}\bullet V_{In}$, and the A$\rightarrow$B transition involves a nearest-neighbor hop of a P atom resulting in the complex $Fe_{In}\bullet V_P\bullet P_{In}$ for the B configuration (Fig. 4). The B1 emission is attributed to the (=/-) transition of Fe_{In} and the B2 emission is the (0/+) transition of V_P. The results in the Table are found to be consistent with the predictions of the model and with first-principles calculations for the appropriate defects in InP.

Significance—Configurational bistability is undoubtedly a manifestation of strong electron-lattice interactions and accompanying large lattice relaxations. By pressure we can continuously tune the strength of these interactions and thereby modify the balance of forces that determine the stability and nature of the different configurations. The present results attest to the value of the pressure variable.

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Contact: G. A. Samara, Physics & Chemistry of Materials, Dept. 1130
Phone: (505) 844-6653, Fax: (505) 844-4045, E-mail: gasamar@sandia.gov

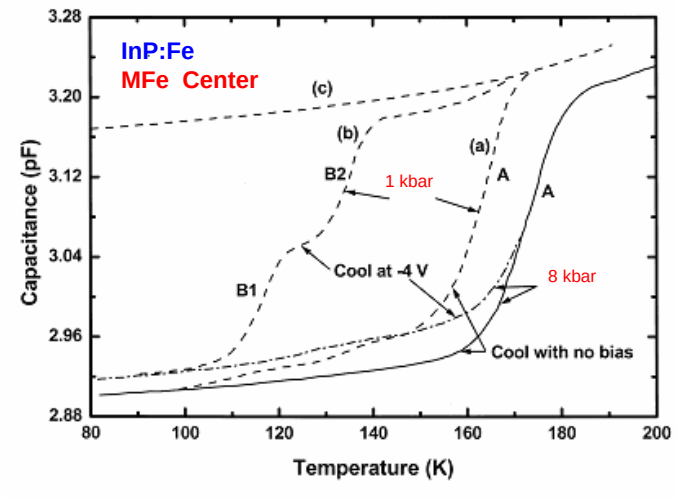

Figure 1. Thermally-Stimulated Capacitance (TSCAP) spectra for the A and B configurations of the MFe center in InP at 1 bar and 8 kbar.

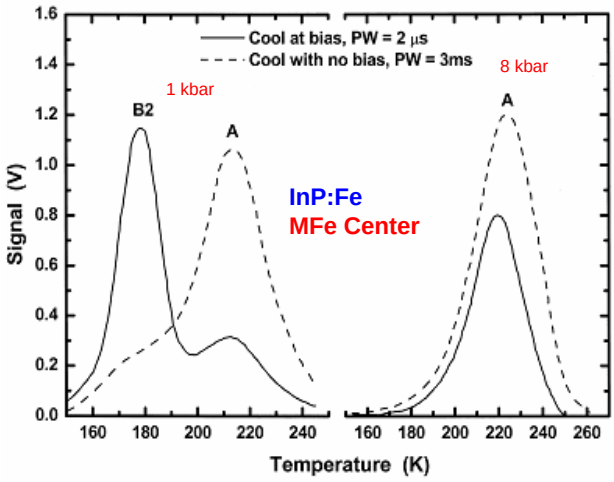

Figure 2. DLTS spectra for the A and B configurations of the MFe center in InP at 1 bar and 8 kbar. The B1 transition is not seen for the conditions of this experiment.

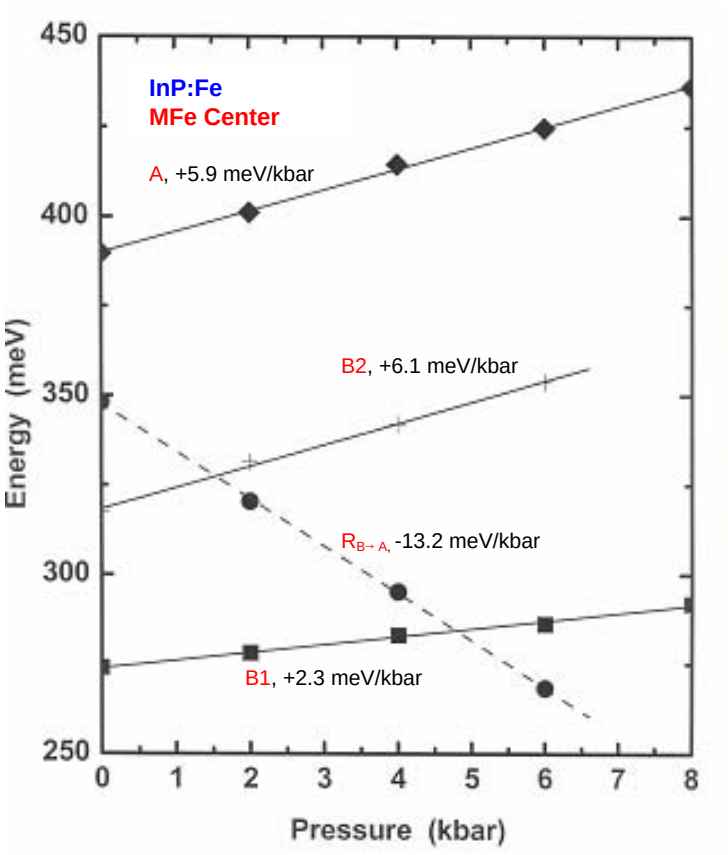

Figure 3. Pressure dependences of the measured electron emission enthalpies, ΔH_n, for the A, B1 and B2 deep levels of the MFe center in InP and of the enthalpy (or activation energy) for the $B \rightarrow A$ transformation.

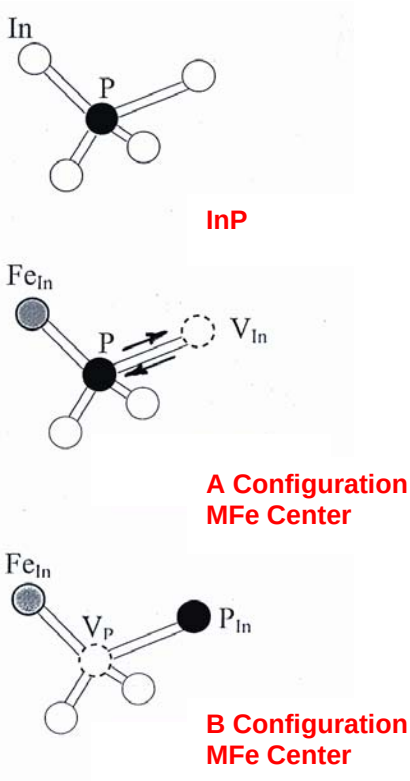

Figure 4. Atomic configurations of InP and of the A and B configurations of the MFe center according to the model described in the text.