Atomic Origin of Magnetic Hardness in our Best Permanent Magnet*

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Abstract. After a brief overview of the Advanced Photon Source, the nation's most brilliant x-ray source for research, we will discuss the atomic origin of magnetic hardness in our best permanent magnet – Nd2Fe14B. Rare-earth (RE) ions dramatically enhance magnetic stability through the interaction of their anisotropic (4f) electron clouds with the electric field of surrounding charges. Here we show that the simultaneous presence of RE ions in dissimilar atomic environments undermines the intrinsic stability of the highest performance permanent magnets. Experiments were done by using helicity-dependent resonant diffraction technique in combination with a digital lock-in detection scheme that synchronizes the measured x-ray diffracted intensity with the helicity modulation of the incoming x-ray beam. Our results, supported by theory, show that unequal neodymium sites in the unit cell of a neodymium-iron-boron single crystal prefer local magnetic moment orientations orthogonal to one another, reducing magnetic stability. These findings highlight the need for manipulating the local atomic structure around rare-earth ions for complete optimization of future magnets.

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