

Abstract Submitted  
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**Deciphering chemical order/disorder and magnetic properties of FePt nanoparticle at the single-atom level** YONGSOO YANG, RUI XU, ALAN PRYOR JR., LI WU, JIHAN ZHOU, JIANWEI MIAO, University of California, Los Angeles, CHIEN-CHUN CHEN, National Sun Yatsen University, Taiwan, M. C. SCOTT, COLIN OPHUS, PETER ERCIUS, Lawrence Berkeley National Laboratory, FAN SUN, HAO ZENG, University at Buffalo, W. THEIS, University of Birmingham, UK, MARKUS EISENBACH, PAUL R. C. KENT, Oak Ridge National Laboratory, RENAT F. SABIRIANOV, University of Nebraska at Omaha — Iron-Platinum (FePt) alloy exhibits large magnetocrystalline anisotropy energy (MAE) with prominent potential for magnetic storage media application. However, a full 3D atomic structure determination of real system has not been accomplished, therefore a fundamental understanding of their magnetic properties remains elusive. Here, we determined the 3D coordinates of 6,569 iron and 16,627 platinum atoms in a model FePt nanoparticle system with 22 pm precision via atomic electron tomography. We identified rich structural variety and chemical order/disorder including 3D atomic composition, grain boundaries, anti-phase boundaries, anti-site point defects and swap defects. The atomic structure was used as direct input for first principles calculations to determine atomic magnetic moments and local MAE. This work not only opens the door to determining 3D atomic arrangements and chemical order/disorder of a wide range of nanostructured materials, but also will transform our understanding of structure-property relationships at the most fundamental level [arXiv:1607.02051].

Yongsoo Yang  
University of California, Los Angeles

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