

Abstract Submitted  
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**The magnetism of TiN** BARBARA JONES, IBM Almaden Res Ctr, CHIUNG-YUAN LIN, SZU-WEN YANG, National Chaio Tung University, Taiwan, PUSHPA RAGHANI, Boise State University, SHRUBA GANGOPADHYAY, University of California Davis — Titanium Nitride is a well-known technological material, used typically in thin 3 micron coatings, in which form it is an extremely hard ceramic. It is the most common PVD coating used today. It shows no evidence of magnetism. We have studied isolated atoms of Ti on a CuN/Cu surface, layers of TiN on a Cu surface, and isolated monolayers of TiN, using first-principles density functional theory (DFT). In all of these geometries, TiN is magnetic, its interactions mainly governed by superexchange, resulting in striped magnetic structures. The question of how this dramatic magnetism disappears as more layers are added and TiN approaches bulk is one we have studied using DFT. We discuss the process by which the magnetism of TiN makes the transition between nanoscale and bulk.

Barbara Jones  
IBM Almaden Res Ctr

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