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Structural and magnetic characteristics of pure NiS_2 in the pressure induced Mott insulator-metal transition YEJUN FENG, Argonne National Laboratory, R. JARAMILLO, Harvard University, A. BANERJEE, T.F. ROSENBAUM, Univ. of Chicago, J.M. HONIG, Purdue University — NiS_2 is a Mott insulator with a half-filled e_g band split by Coulomb repulsion of Ni d electrons. The low temperature insulator exhibits two types of coexisting antiferromagnetic order (M1, M2), but the connection between the magnetism and electron correlations is not well understood. Using high-resolution x-ray diffraction in a diamond anvil cell, we probe both the lattice and M2 magnetic structures of pure NiS_2 across the pressure induced insulator-metal transition at T = 3.5 K. Unlike most Mott systems, which have reduced symmetry in the insulating phase, we find that the high pressure metallic state of NiS_2 is the phase with reduced symmetry. The M2 antiferromagnetism disappears along with the high symmetry phase at high pressure. Our observations suggest that the M2 antiferromagnetism arises from a super-exchange interaction between correlated electrons in the Mott insulating phase.

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