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Microscopic Structure of Mn Atom Chains on the Si(001) Surface Investigated by Scanning Tunneling Microscopy A. FUHRER, F. J. RUEß, N. MOLL, A. CURIONI, D. WIDMER, IBM Research, Zürich Research Laboratory, Säumerstrasse 4, 8803 Rüschlikon — The Si(001) 2x1 reconstructed surface has the interesting property that many metal atom species form nearly perfect 1D atomic wires oriented perpendicular to the Si dimer rows during deposition at room temperature. These wires are thought to consist of metal dimers located between the dimer rows linking up to form atomic chains. More recent experiments indicated that similar wire formation occurs for Mn which, with its half filled d-shell, has interesting magnetic properties e.g. when used as a dopant in dilute magnetic semiconductors. In our experiments we use scanning tunneling microscopy to study the atomic structure of these Mn-wires in detail and find that it is different from that of the other known metal wires. We show that two distinct types of Mn wires occur, with an asymmetric appearance relative to the underlying Si lattice. While one type of asymmetry can be linked to the buckling of the Si dimers near the Mn-wires the other is found to be intrinsic to the microscopic structure of the Mn-wires. We further compare high-resolution bias-dependent constant current images with images simulated for a Mn trimer wire structure using density functional calculations employing the CPMD code.

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