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Role of Anomalous Channeling on HAADF in a Quasi-1D KMn_6Bi_5 Structure

Hee Joon Jung[1], Jin-Ke Bao[2], Duck Young Chung[2], Mercouri G. Kanatzidis[2,3] and Vinayak P. Dravid[1]

[1]Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208, USA
[2]Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA
[3]Department of Chemistry, Northwestern University, Evanston, Illinois 60208, USA

One-dimensional (1D) structures reveal unconventional properties such as topological spin excitation [1], Luttinger liquid with spin-charge separation [2], charge density wave induced by Peierls instability [3]. Because the perfect 1D structure is rare in nature and observation along the 1D chain direction is problematic using TEM, quasi-one-dimensional (Q1D) compounds with atomic or molecular chains bundled into two-dimension (2D) [4] can show exceptional properties obtainable in an ideal 1D system. KMn_6Bi_5 is a Q1D structure, a unique 2D array of one-dimensional $[Mn_6Bi_5]^-$ nanowire (NW) along the *b* axis shown in Fig. 1, has monoclinic space group $C2/m$ with a = 22.994 Å, b = 4.6128 Å, c = 13.383 Å and β = 124.578°. Each $[Mn_6Bi_5]^-$ NW (diameter≈8.7 Å) is composed of a Bi nanotube (NT) shell surrounding a Mn nanorod (NR) core. While the Bi NT consists of Bi pentagons stacked along b axis, the Mn NR consists of outer Mn pentagon caging a 1D Mn atomic straight chain at center along the *b* axis. Because 2_1 screw axis is located on the center 1D Mn, the atomic density of the center Mn column have effectively two times higher than that of outer Bi and Mn atomic columns as shown in Fig. 1. The HAADF contrast provides interpretable Z-contrast collecting incoherently high-scattered elastic electrons. However, electron channeling (EC) on uniquely isolated one-dimensional (1D) atomic column acting as 1D electron waveguide can disturb straightforward interpretation of experimental Z-dependent HAADF contrast.

Here we present a Q1D KMn_6Bi_5 has 2D-arrayed 1D $[Mn_6Bi_5]^-$ nanowire along the *b* axis, which is a Bi nanotube shell wrapping Mn core nanorod composed of 1D central Mn atomic column embraced by outer helical Mn pentagonal columns (2_1 screwed), and it shows lower HAADF contrast on the center 1D Mn than that of outer Mn as can be seen in Fig. 2 even though the center has 2 times higher atomic density than the outer. Extraordinary discrepancy was investigated by multislice simulation telling that thickness-dependent electron channeling of the central 1D Mn is different from that of the outer Mn. Furthermore, reverse annular bright field (RABF), simply inverses the contrast of ABF, reveals complementary information to the HAADF. This result from the QID delivers a new understanding of the occurrence and consequences of channeling or de-channeling phenomena under which their influence is strengthened or weakened over the thickness.

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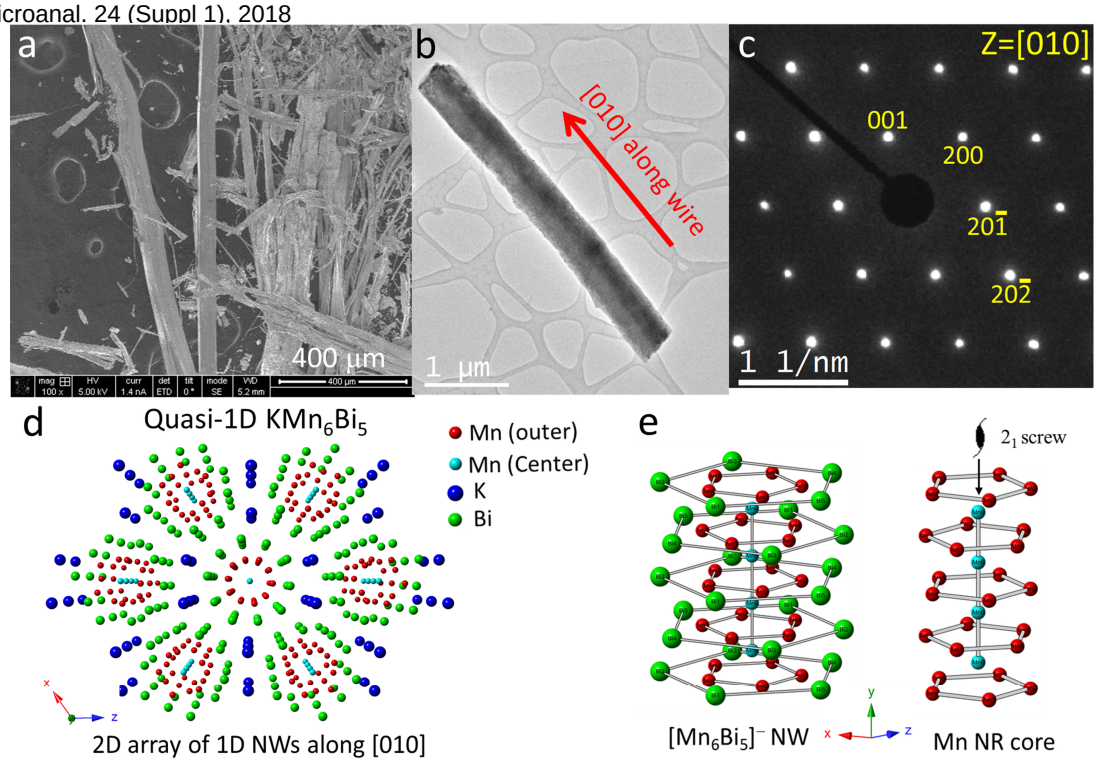

Figure 1. a, b SEM and BFTEM of KMn_6Bi_5 NWs. c. Diffraction from [010] zone axis. d, e. Schematic figures of Q1D KMn_6Bi_5: 2D array of 1D $[Mn_6Bi_5]^-$ nanowires and each $[Mn_6Bi_5]$- nanowire is composed of an outer pentagonal Bi nanotube (2_1 screwed) wrapping a center Mn nanorod. The center nanorod is also composed of a central 1D Mn straight chain caged by pentagonal Mn nanotube (2_1 screwed).

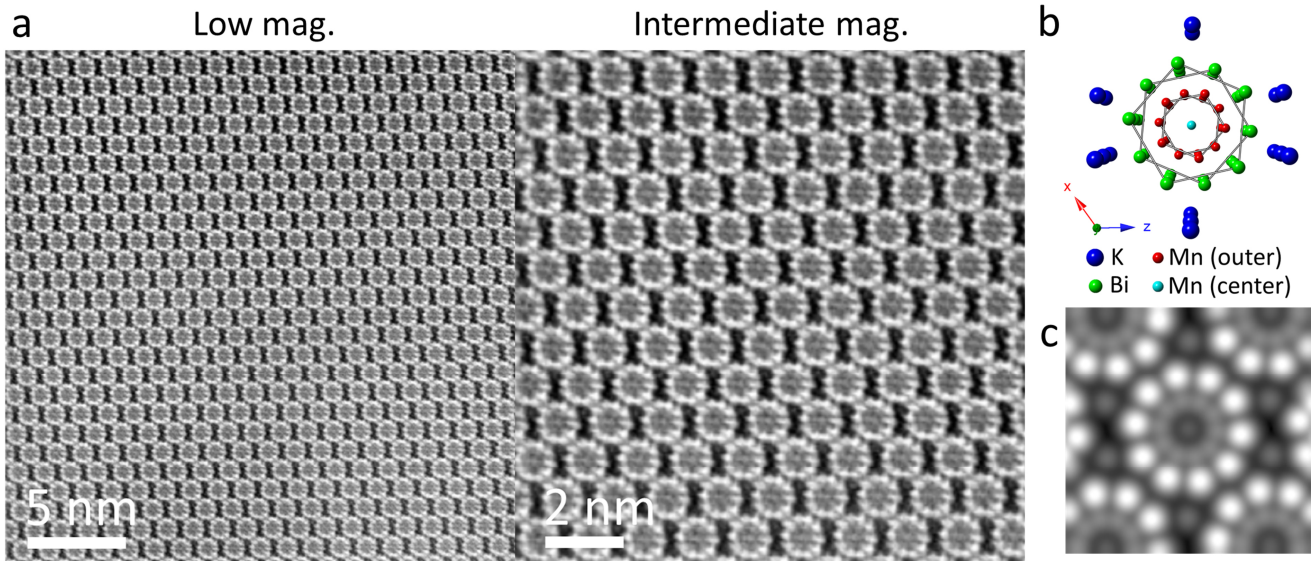

Figure 2. a. HAADF images of Q1D KMn_6Bi_5 showing well-bundled 2D array of 1D $[Mn_6Bi_5]^-$ NWs. b. Schematic of each $[Mn_6Bi_5]$- nanowire with K atoms. c. Multislice HAADF simulation of the Q1D KMn_6Bi_5.

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