Abstract Submitted
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Ab initio investigation of thermoelectric properties of AlN nanowires under axial stress[1] GEORGE ALEXANDRU NEMNES, TUDOR LUCA MITRAN, ADELA NICOLAEV, University of Bucharest, Faculty of Physics, "Materials and devices for Electronics and Optoelectronics" Research Center, CAMELIA VISAN, Horia Hulubei National Institute of Physics and Nuclear Engineering, The Department of Computational Physics and Information Technologies, LUCIAN ION, STEFAN ANTOHE, University of Bucharest, Faculty of Physics, "Materials and devices for Electronics and Optoelectronics" Research Center — Small diameter nanowires, down to a few lattice constants, are structurally and electronically different from bulk, due to the large surface-to-volume ratio and the effects of the surface states, which has consequences in the optical absorption and in the electrical/thermal transport. It has been recently established that AlN nanowires can suffer a stress induced phase transition from a wurtzite to a graphite-like phase [1]. The thermopower of atomic-sized wurtzite AlN wires coupled to Al(111) bulk contacts is investigated at low temperatures using Green-Keldysh formalism. We ?nd that the conduction of the wide bandgap semiconductor wire is essentially enhanced by the presence of surface states. We show that the evanescent coupling to the surface states is strong enough to render thermopower of a few tens of micro-V/K, which may be enhanced by controlling the position of the surface states. [2]. We also investigate the changes in the thermopower under applied axial stress, comparatively analyzing the nanowires in the wurtzite and graphite-like configurations. [1] T.L. Mitran, Adela Nicolaev, G.A. Nemnes, L. Ion, S. Antohe, Comput. Mat. Sci. 50, 2955 (2011) [2] G.A. Nemnes, C. Visan, S. Antohe, Physica E 44, 1092 (2012)

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