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Critical Behaviors in Pb(Zr,Ti)O_3 Ultrathin films EMAD ALMAHMOUD, IGOR KORNEV, LAURENT BELLAICHE, Physics Department, University of Arkansas, Fayetteville, Arkansas 72701, USA — The first-principles-derived approach of Ref.[1] is used to determine the thickness dependency of Curie temperature and of the spontaneous polarization in Pb(Zr,Ti)O_3 (PZT) thin films that are under stress-free and open-circuit boundary conditions. It is found that, above a thickness of 7 (B-)monolayers (ML), the Curie temperature follows the finite-size relation of Ref.[2] with a critical exponent $\lambda = 1.04$. On the other hand, the Curie temperature deviates from this "usual" relationship for thickness of 6 monolayers and below, characterizing a crossover from a three- to a two-dimensional behavior. This striking crossover is also reflected in the critical exponent β, that is associated with the power law describing the behavior of the polarization with thickness. As a matter of fact, such exponent decreases drastically from 0.14 to 0.1 between 7 and 4 ML. This work is supported by ONR grants N 00014-01-1-0365, N00014-04-1-0413 and 00014-01-1-0600, by NSF grants DMR-0404335 and DMR-9983678, and by DOE grant DE-FG02-05ER46188.

[1] E. Almahmoud, Y. Navtsenya, I. Kornev, H. X. Fu, and L. Bellaiche, *Phys. Rev. B 70, 220102® (2004)*

[2] G. A. T. Allan, Phys. Rev. B1, 352 (1970).

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