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Local dielectric permittivity profiles of sapphire/polypropylene interfaces LIPING YU, V. RANJAN, M. BUONGIORNO NARDELLI, J. BERNHOLC, NC State U — Recently, the need for high-power-density capacitors has stimulated research to develop composite dielectric materials with high-k nanoparticles embedded in a polymer matrix. In these materials, surfaces and interfaces may play an important role in determining the overall dielectric properties. We present first-principles investigations of the dielectric permittivity profiles across slabs and interfaces of sapphire(α -Al₂O₃)/isotactic-polypropylene(iPP). Our results indicate that the permittivity profile at interface strongly depends on the nanoscale averaging procedure. We propose an averaging model that ensures near-locality of the dielectric function. We find that: (i) the dielectric permittivity approaches the corresponding bulk value just a few atomic layers away from the interface or surface; (ii) the dielectric constant is enhanced at the surfaces of the isolated α -Al₂O₃ slabs, while no enhancement is observed at the iPP slab surfaces; and (iii) the dielectric transition at the α Al₂O₃/iPP is mainly confined in the α Al₂O₃ side.

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