An interface formulation for the Poisson equation in the presence of a semiconducting single-layer material

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Single-layer materials such as graphene are promising for various applications, in particular to optimize electronic devices. For instance, 2D semiconductor materials allow to design transistors with channel thickness on the atomic scale. In this context, we are interested in performing self-consistent computations to study the transport of electrons in devices such as a graphene field-effect transistor. In this work, we concentrate on the numerical resolution of the Poisson equation proposing to model the single-layer structure as an interface. More precisely, we consider a device with an active zone made of a single-layer material sandwiched between two thick insulator regions (oxide). The associated Poisson equation is characterized by both a surface particle density and an out-of-plane dielectric permittivity exhibited in a region of effective dielectric thickness surrounding the single-layer material, as emphasized in [1]. To avoid mesh refinements, we derive an interface problem based on the natural domain decomposition suggested by the physical device, averaging the potential across the dielectric effective region. It is inspired by [2] where this approach is used to model fractures in porous media. We obtain two Laplace equations in the oxide subdomains coupled with an effective Poisson equation on the interface with an extra source term that represents the contribution of the surrounding environment to the channel material. After a presentation of the interface model, we discuss its discretization with a finite element method, using the so-called three-fields formulation, where the weak continuity between the oxide subdomains and the interface is imposed by means of Lagrange multipliers following [3]. Interestingly, the interface discretization does not need to match with the one of the subdomains and we take advantage of this flexibility in the numerical experiments we are performing to illustrate the approach.

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References

[1] J. Fang, W.G. Vandenberghe, M.V. Fischetti, Microscopic dielectric permittivities of graphene nanoribbons and graphene, *Phys. Rev. B*, **94** (2016), 045318.

[2] C. Alboin, J. Jaffr, J.E. Roberts and C. Serres, Modeling fractures as interfaces for flow and transport in porous media, in Fluid flow and transport in porous media, *Amer. Math. Soc.*, **295** (2002), 13-24.

[3] S. Bertoluzza, Analysis of a stabilized three-fields domain decomposition method, *Numer. Math.*, **93** (2003), 611634..