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Calculation of the Effective Diffusion Coefficient for Heterogeneous Media

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1 Introduction

In this paper we discuss the range of the applicability of our recent approach [1] for the effective diffusion coefficient (mobility) in two-phase systems, e.g. composite materials, porous media, polymer blends, matrices with inclusions. We derived the equation for D_{eff} as a function of the partial diffusion coefficients of a defect (or probe particle) in inclusions, D_1, with the fractional concentration Φ=0...1, and the diffusion coefficient in the host matrix, D_2, taking into account the energy barrier for the particle penetration into an inclusion. We compare our results with previous theories, starting with the generally–accepted Maxwell-Garnett formula [2] and finishing with very recent studies [3].

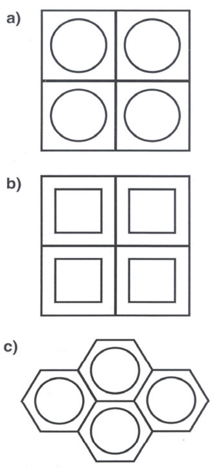

Fig.1. Inclusions of different shapes

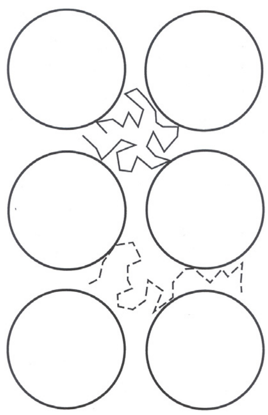

Fig.2. Pocket effect of particle trapping

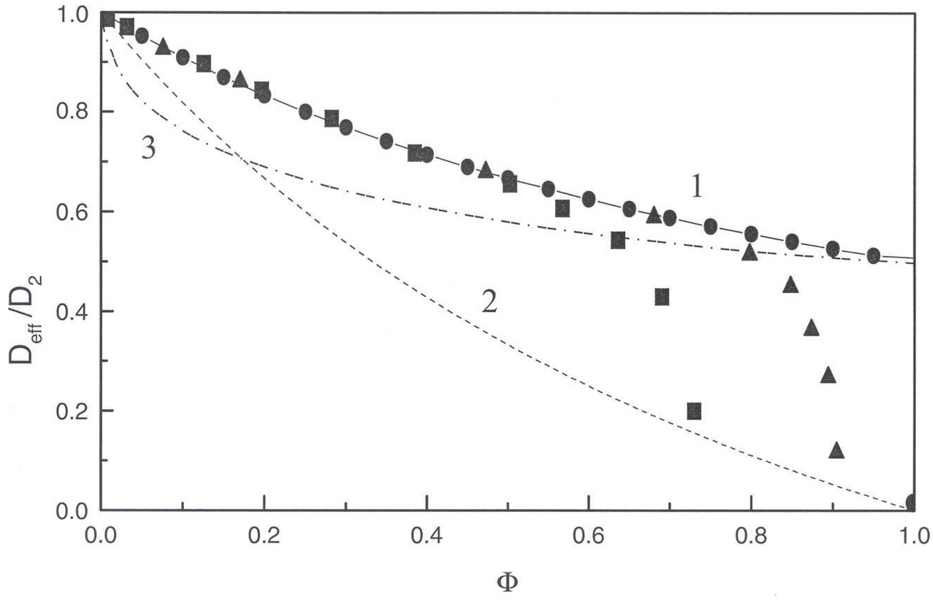

Fig.3. A comparison of our theory (curve 1) with Maxwell-Garnett eq. (curve 2) and eq.(14) from Ref. (3) with 2D MC simulations for periodically distributed impenetrable inclusions as a function of their dimesionless concentration Φ. Square symbols are spherical inclusions on a square lattice; triangles spherical inclusions on a hexagonal lattice; and full circles square inclusions on a square lattice (see Fig.1).

2 Monte Carlo simulations

We performed 2D Monte Carlo computer simulations, in order to test the validity of the various equations. They demonstrate that our mean-field theory [1] reproduces surprisingly well results for square-shaped inclusions without concentration limitation. For inclusion with other shapes there are critical fractional concentrations at which particles become trapped in pockets between inclusions (Fig.2).

3 Conclusions

The standard Maxwell-Garnett equation gives wrong concentration dependence for impenetrable inclusions, by reasons discussed in our paper [1], however, its extension gives excellent results. We discuss disadvantages of the approach presented in Ref. [3] which reproduces correctly two limiting cases, but is not accurate at intermediate concentrations of inclusions (curve 3 in Fig.3).

References

[1] J.R. Kalnin, E.A. Kotomin, and J. Maier, J. Phys. Chem. Sol. **63**, 449-456 (2002).
[2] J.C. Maxwell-Garnett, Phil. Trans. R. Soc. London, **203**, 385 (1904).
[3] I.V. Belova and G.E. Murch, J. Phys. Chem. Sol. **64**, 873-878 (2003).