Orientation of liquid crystals on interface

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Application of oligomethylsiloxane (ODMS) in optical and electrooptic devices is very attractive because of its high elasticity, adhesion capacity and other mechanical properties as well as its stability to ambient conditions [1-3]. In this paper the interaction of mesogen molecules with the ODMS surface is considered using the atom-atom potentials method. The calculated interaction energy value is essentially higher than experimentally obtained values of azimuthal and polar anchoring energy. This fact is in agreement with results obtained earlier [4-6]. To describe properties of the LC near the interface we use a model that explains the observed values of azimuthal and polar anchoring energy. Calculations were performed by using of two methods. The first is the atom-atom potentials method:

\[ E = \sum_{i,j} \left( \frac{A}{R_{i,j}^2} + \frac{B}{R_{i,j}^6} \right) \]

\((R_{ij})\) is a distance between \(i\)-th and \(j\)-th atoms, \(A\) and \(B\) are constants). In the second a potential of interaction of two rod-like molecules proposed by us is used:

\[ E = \frac{a^3 + 3ab^2 \cos^2 \varphi}{(a^2 - b^2 \cos^2 \varphi)^3} \]

\((\varphi)\) is an angle between interacting molecules; \(a, b\) are constants.

The dependence of the interaction energy on polar and azimuthal angles defining the orientation of mesogen molecules towards the surface layer of planar oriented nematic liquid crystal was obtained.

Results obtained by both methods are rather close one to another, to other theoretical simulations and to experimental values of azimuthal and polar anchoring energy [7-10].

The potential proposed here can be used for any systems consisting of rod-like molecules.

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References

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