ABSTRACT

The cooling behaviour of the generic Gay-Berne model consisting of 500 particles with its original parameters ($\epsilon_{ss}/\epsilon_{ee} = 5$, $\sigma_{ss}/\sigma_{ee} = 3$, $\nu = 1$, $\mu = 2$) was studied at constant pressure using Monte- Carlo simulation technique. Simulation on such system had been conducted previously but the system was heated from the ordered phase into the isotropic phase. In this report results from both these works will be discussed and where appropriate comparison will be made. Several phases were observed including isotropic and smectic, depending on the temperature and pressure of the system understudied. The structure of the smectic phase was characterised and it was found to be of a smectic hexatic B phase. These smectic layers were found to be interdigitated with the smectic layer thickness found to be much less than the length of the molecules. Moreover they were also found to be considerably tilted with respect to the layer's normal. The thermodynamic properties of this system were also calculated as a function of reduced temperatures. Sinces these results were obtained at constant pressure, direct comparison can be made with the behaviour of real mesogens which were studied under the same condition. The system also display a notable histeresis behaviour over the region of isotropic - smectic B transition whereby it experienced a considerable supercooling and superheating. We have also attempted to measure Monte-Carlo " time " by relating the maximum displacement parameter to the average speed of a typical real system like PAA. The calculated "time - step" and those obtained from others simulated time steps were found to be in a consistent agreement.

ABSTRAK

Kajian penyejukan sistem model generik Gay- Berne yang mengandungi 500 molekul dengan menggunakan parameter-parameter asalnya ($\epsilon_{ss}/\epsilon_{ee} = 5$, $\sigma_{ss}/\sigma_{ee} = 3$, $\nu = 1$, $\mu = 2$) telah dijalankan dibawah tekanan tetap dengan menggunakan teknik simulasi Monte - carlo. Penyelidikan seperti ini pernah dilakukan terdahulu tetapi hanya tertumpu kepada pemanasan sistem dari fasa tersusun hingga ke fasa isotropik. Walaubagaimana laporan ini akan memberikan perbincangan serta perbandingan bagi kedua-dua kajian tersebut. Beberapa fasa utama telah ditemui termasuklah isotropik dan smektik, bergantung kepada tekanan dan suhu yang dikenakan kepada sistem. Setelah meneliti struktur fasa selanjutnya didapati bahawa fasa smektik adalah merupakan fasa smektik hexatik B. Kajian ini juga menunjukan bahawa lapisan smektik bertindihan (interdigitated) memandangkan nilai tebal lapisan adalah lebih kecil dari panjang molekul. Tambahan pula terdapat bukti yang menunjukan bahawa lapisan smektik ini condong (tilted) berbanding dengan normal lapisan. Semua sifat-sifat termodinamik telah dikira bersandarkan fungsi suhu berskala. Oleh kerana keputusan yang diperolehi adalah hasil kajian dibawah tekanan tetap, maka perbandingan terus boleh dibuat dengan sifat-sifat mesogen senenar yang telah diukur pada keadaan yang serupa. Terdapat juga fenomena "histeresis" pada takat peralihan isotropik-smektik yang mana sistem mengalami kelakuan pemanasan lampau dan penyejukan lampau. Pengiraan "masa" Monte-Carlo juga dikira dengan menghubungkaitkan nilai parameter putaran maksimum denngan purata halaju bagi sistem hakiki seperti PAA. Keputusan pengiraan masa tersebut didapati hampir menyetujui dengan pengiraan bagi masa dari kaedah lain.