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Surface Science 538 (2003) 30–44
SURFACE SCIENCE
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# Simulated behavior of krypton/argon mixtures confined between two graphite slabs: new terrain for familiar systems

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Received 1 November 2002; accepted for publication 14 April 2003

**Abstract**

We present the results of $(N, \rho, T)$ molecular-dynamics simulations of krypton/argon mixtures confined between two graphite slabs with varying spacing. Structural, thermodynamic and bond-orientational quantities indicate a group of new phases and phase transitions for these already well-explored systems, and they also further delineate the close cooperation of vertical atomic motion and melting in adsorbed systems. For pure argon and systems with a high argon fraction we observe commensurate and rotated phases. Commensurate argon is stabilized over a wide temperature range for certain slab spacings, and high-temperature solid phases exist for all mixture fractions studied. For all systems explored two phenomena are observed: (1) the melting temperature $T_m$ of the system may be controlled to a fairly precise degree within a certain range by only the slab spacing, and (2) competing effects of confinement and heightened room for in-plane atomic fluctuations due to enhanced vertical fluctuations causes $T_m$ to reach a minimum value as the slab spacing is varied. The effects of varying the mixture fraction are also explored and, although emphasis is placed on melting, evidence of confinement-induced and composition-induced phase transitions is given and briefly discussed.


*Keywords:* Surface melting; Molecular dynamics; Noble gases; Graphite; Physical adsorption

## 1. Introduction

Rare gases adsorbed on a graphite substrate have received attention in basic and applied research areas for decades [1]. Krypton [2–16] and argon [17–29] on graphite have both been studied extensively and exhibit interesting and unique behavior. With the realization of nanoscale systems with non-planar geometries and with our increasing degree of control over them, interest in the behavior of familiar systems (such as planar adsorbates) in confined geometries continues.

There are molecular simulation studies of various types of fluids interacting with planar surfaces which provide a time-dependent potential that can be used to conduct constant pressure simulations [30], of the solvation force between two planar surfaces separated by a confined liquid [31], of osmotic stress in confined colloid/solvent mixtures

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doi:10.1016/S0039-6028(03)00574-0