This project is a study of the behavior of physisorbed monolayers of Xe on Pt(111) surfaces. We investigated various characteristics of the system such as lattice structure, domain wall formation, thermodynamic and scattering properties, phase transitions and the ground state energy.

It is a goal of this research to relate the results of the computer simulation to the experimental results found in the literature, testing and establishing the applicability of our model and to develop a reliable model of physisorption that correctly explains and predicts the results encountered in nature.

**RESULTS AND DISCUSSIONS**

**Lattice Configuration and Wall Formation**

The graphs below illustrate the configuration of the xenon atoms at different temperatures, where each color represents one site in the six-fold hexagonal symmetry and the black spots are the domain walls.

**Phase Transition**

The melting of the Xe monolayer was observed using the Nelson-Halperin order parameter (NHOP) [2], a measure of how the local ordered hexagonal structure is propagated across the lattice and how it varies as a function of temperature. Not only did we find that the transition was continuous with a very smooth curve, but also the melting temperature is much higher than the one for xenon alone (T=100K). This indicates that the substrate has a very strong influence on the system and the coefficients calculated for our potential could be too high. First, we initialize the system at very cold temperatures and heated it up during melting until the whole system was liquid (or gas from the initial configuration). After that we cooled the system back down through solidification until we reached again the lowest possible temperature. The difference between the cooling and the heating path in Fig. 02 indicates hysteresis in the system which appears to be in a meta-stable state.

**METHODS**

The method chosen was molecular dynamics simulations and our theoretical model was the Barker-Rettner model [1] with the HFD-B2 plus McLachlan interactions [2]. We simulated a monolayer (single atom thick 2-dimensional layer) of solid xenon adsorbed on a platinum surface, which acts as the potential field for the xenon adatoms. The adsorption site is considered to be the A-top site (right above the platinum atom) and no 3-dimensional motion is allowed aside of the variation in the optimal distance from the substrate over the surface. The first studied system was constrained with approximately 4,000 particles with different densities around and at the registered phase. The second system was formed by approximately 20,000 particles and composed an unconstrained island of xenon surrounded by 2-dimensional Xe gas that was allowed to rotate and expand/contract on top of the substrate.

**RESULTS AND DISCUSSIONS**

**Lattice Parameter**

A number of different techniques were used to calculate the lattice parameter of the Xe in the process of defining which method would provide more accurately the lattice constant. A large part of the project was dedicated to this task and the 2K system was used for this purpose only. We tested methods based on the pair distribution function, density profile calculations and structure factor calculations. We found that even though they all provided good results at low temperatures, the structure factor calculations was more reliable over the whole observed range of temperature. A set of numerous sorting and fitting routines were created to analyze the structure factor calculations and find the best value for the location of the peak in reciprocal lattice space. From this result we were able to calculate an accurate value for the lattice parameter. The result for the 4K system was 4.79 Å at the registered phase and the same for the 20K system. All following results are related to the 20K system.

**Phase Transition**

The melting of the Xe monolayer was observed using the Nelson-Halperin order parameter (NHOP) [2], a measure of how the local ordered hexagonal structure is propagated across the lattice and how it varies as a function of temperature. Not only did we find that the transition was continuous with a very smooth curve, but also the melting temperature is much higher than the one for xenon alone (T=100K). This indicates that the substrate has a very strong influence on the system and the coefficients calculated for our potential could be too high. First, we initialize the system at very cold temperatures and heated it up during melting until the whole system was liquid (or gas from the initial configuration). After that we cooled the system back down through solidification until we reached again the lowest possible temperature. The difference between the cooling and the heating path in Fig. 02 indicates hysteresis in the system which appears to be in a meta-stable state.

**Ground State Energy and Further Discussions**

The 20K system was initialized at different rotation angles from 0 to 30° in respect to the f3xv3R30° structure and in all cases the particles rotated back to the aligned configuration in only a few time steps. However, instead of the whole patch rotating back to 0 while maintaining the hexagonal form, the boundaries did not move and the atoms realigned in respect to each other. This contrasts with the Xe adsorbed on graphite system, which is being studied in another project, where the patch rotated as a whole. That also indicates strong substrate-adlayer interaction.

The simulation had long relaxation times and in the time range available in the simulation it was not possible to reach true thermodynamic equilibrium. One possible interpretation is that the system could be trapped in a meta-stable state. After the solidification, the Xe atoms regrouped in numerous patches, each much smaller than the initial island. This structure was found to have a slightly higher energy than the initial configuration. The registered phase is definitely the ground state of the system.

**CONCLUSION**

At the end of this phase in our simulation, we have reached the conclusion that either the potential used in these calculations is too strong and therefore lowering it would lead as to results that match the experiments or we could have encountered a better interpretation to the experimental observations than the ones in the literature. New simulations with a different coefficients are being run to refine our hypotheses and build a model that better relates to reality.

**Bibliographic References**


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