

SBIR 06.2 PHASE I - AWARD DETAILS	
ORGANIZATION	ARL
TOPIC NUMBER	A06-075
CONTRACT NUMBER	
YEAR OF AWARD	
AWARD START DATE	
AWARD COMPLETION DATE	
PROPOSAL NUMBER	A062-075-0523
TITLE	Simulation Tools for Strain Engineering, Manufacturing and Design of Novel Optical and Electronic Superlattice Materials and Surfaces
PROJECT MANAGER	Alok Chatterjee (630) 774-0203 alok@epir.com
COMPANY	EPIR Technologies Inc 590 Territorial Drive, Suite B Bolingbrook IL 60440-4881 Minority Owned: No Veteran Owned: No Number of Employees: 18
KEYWORDS	InGaN/GaN, Quantum dots, Molecular Dynamics, simulations, electronic structure.
ABSTRACT	The overall objective of this Phase I proposal is to create a model based on molecular dynamics (MD) that can predict the specific Quantum Dot Superlattice (QDSL) heteroepitaxial structures that will grow, given various factors such as growth temperature, flux rate, and spacer thickness. AlGaIn/GaN heterostructures have attracted a great deal of theoretical and experimental interest because of their applications in high-power microwave devices, in high-frequency field effect transistors and in blue light-emitting diodes, among others. Specifically, ab-initio density functional theory calculations will be performed to determine accurate parameters for the interatomic potentials to be employed in MD growth simulations. Next, potentials such as the Rockett and modified Stillinger-Weber potentials will be investigated for their suitability. Once the potential parameters have been optimized, MD simulations of the growth of InGaN/GaN QDSL heterostructures will be performed. After the simulated growth of each InGaN/GaN QDSL layer, the system will be allowed to equilibrate. Defect formation will be studied as the growth proceeds. The strain in these simulated structures will be calculated. The effect of strain on the electronic structure of InGaN/GaN QDSL structures will also be calculated. Finally, the tradeoffs in the choice of growth parameters will be explored.
BENEFITS	The ability to predict crystal quality and material performance will improve and allow innovation in the production of III-V QDSL's. EPIR plans to commercialize the models created in this proposed effort by developing a user-friendly software package. This software will have the ability for the user to enter various growth parameters and material properties and observe the effect of varying the input parameters to obtain the desired material performance.