MS.27.5

Acta Cryst. (2011) A**67,** C73

Comparison of surface fractal features of thermophilic and mesophilic proteins

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Understanding the adaptation of proteins to high temperature continues to be a subject of intense study. Several factors have been proposed as contributing to protein thermo stability and it is of interest to understand the interplay of the factors causing stability at high temperature. Surface texture is an important structural feature since it plays roles in protein stability, diffusion, protein self-association, recognition of different subunits, macromolecules and ligands. Different types of structural and geometric patterns are present on the protein surface that are implicated in interactions with other proteins or nucleic acids or ligands or small molecules. Mutations on the surface of a given protein have been used to increase the thermal stability of the protein. Also, interactions forming on the outer surface of a protein are likely to be preferred during the course of evolution. Hence, the quantification of protein surface may yield valuable insights concerning stability and functionality of proteins. However, despite protein surface being important, a quantitative evaluation of surface smoothness of (hyper)thermophilic and mesophilic proteins has not been reported so far prompting us to carry out a comparative investigation of the surface features of different classes of proteins using the concept of fractal geometry. The 3D structures for all the proteins, selected for the analysis, had been determined using X-ray crystallographic methods and were retrieved from the protein data bank (PDB). Structures determined using NMR methods and modeled structures were excluded from the data sets. The dataset was additionally filtered such that upon superposition of corresponding C_α atoms, the root mean square deviation (RMSD) between the (hyper)thermophilic and their homologous mesophilic proteins is not more than 5Å and chain lengths differ by not more than 30 amino acid residues. Here we compared the extent of corrugation or surface smoothness of proteins from (hyper)thermophilic and mesophilic organisms, quantified in terms of surface fractal dimension. The analysis clearly revealed that, moderate thermophilic proteins have significantly lower surface fractal dimension or greater surface smoothness (2.241 versus 2.261, $p = 3.6\times10^{-4}$) than their counterparts from mesophilic organisms in a two tail paired distribution at the 0.05 level. Importantly and unlike several other structural metrics, surface smoothness enables a clean discrimination between proteins from moderate thermophiles and their homologous proteins from mesophilic organisms. Interestingly, for hyperthermophiles, surface smoothness is not significantly different from that of their mesophilic counterparts perhaps suggesting that the strategies adopted by hyperthemophilic proteins to achieve thermostability may be different from those adopted by proteins from moderately thermophilic organisms. This could be a direct consequence of the temperature dependence of various interactions which stabilize proteins. Our analysis strongly suggest that moderate thermophiles and hyperthermophiles should be treated separately in any comparative study concerning thermostability of proteins.The results obtained here could be exploited for the engineering of proteins with increased thermostability for practical applications.

Keywords: fractal, thermophile, mesophile

MS.28.1

Acta Cryst. (2011) A**67,** C73

Controlling stress in GaN-on-Si

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GaN-on-Si heteroepitaxy has become a serious alternative to established growth of group-III-nitrides on sapphire or SiC because of its low price, large diameter wafers, and thermally well conducting properties. Most of the work and published device results have been for GaN growth on (111) silicon substrates. Recently, we have demonstrated thick, crack-free layers exceeding 14 µm in thickness. Meanwhile, big companies as Samsung1 and Bridgelux2 have announced breakthroughs in GaN-on-Si-based high-power LEDs aimed for general lighting. For such application thick, high-quality structures with highly conducting n-type layers are required which is a major challenge because of tensile thermal stress leading to cracks in the GaN/Si system during cooling down. In addition to thermal stress doping with Si is a major source of tensile stress. The latter can be overcome by Ge-doping instead of Si-doping3. We show ways to control stresses and strains in GaN heteroepitaxy to achieve crack-free, device-relevant GaN layers on Si with thicknesses up to >14 µm. New fields are growth of semipolar GaN on high-index Si(h11) substrates as well as the realization of GaN/AllnN based microcavities with InGaN/GaN quantum wells for optoelectronic devices such as a blue VCSELs or a polariton lasers turned in worldwide focus of interest. We have grown first mirror structures on Si substrates. However, the growth of AlInN/GaN DBR layers with perfect interfaces turned out to be much more difficult than expected. With small deviations from the lattice-matching conditions in the order of 1% after a certain thickness of around 30 nm the upper AlInN interfaces become very rough similar to a Stranski-Krastanov transition whereas the lower ones remain flat. The roughness is smoothened by the subsequent GaN layers. This effect occurs in both compressively or tensely strained conditions on sapphire as well as on silicon substrates.

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Keywords: GaN on Silicon, stress control, heteroepitaxy

MS.28.2

Acta Cryst. (2011) A**67,** C73-C74

Diffuse x-ray scattering from defects in GaN epitaxial layers

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GaN epitaxial layers are widely investigated nowadays because of their broad application in electronics and optoelectronics. The limiting parameters of the optoelectronic performance of these materials are their structural quality and densities of various defect types, so that a reliable non-destructive method for the quality assessment of these layers is of a great importance.

In c-oriented wurtzite GaN layers, screw and edge dislocations perpendicular to the surface (threading dislocations) represent the most