Pressure-induced structural transformation of CdSe nanocrystals

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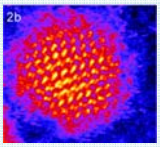
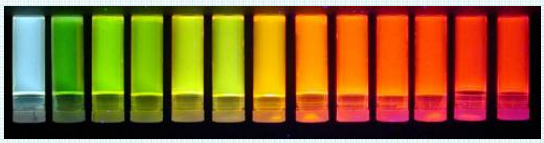
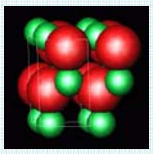
We have studied the pressure-induced structural transformation of CdSe nanocrystals using constant pressure molecular dynamics simulations for finite systems. In agreement with the experiment, it is observed that the process of transformation from wurtzite to rocksalt structure is strongly dependent on the shape and size of the nanocrystals. Upon pressure loading, the spherical CdSe nanocrystals directly transfer to rocksalt structures with nanoscale grain boundary formed, while the faceted ones first transfer to hexagonal MgO structure, and then the rocksalt structure without any grain boundary results.



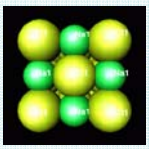


Semiconductor nanocrystals, also known as "quantum dots", maintain the crystalline structure of the bulk. Due to the finite size, the physical properties of theses materials may change significantly compared to the bulk

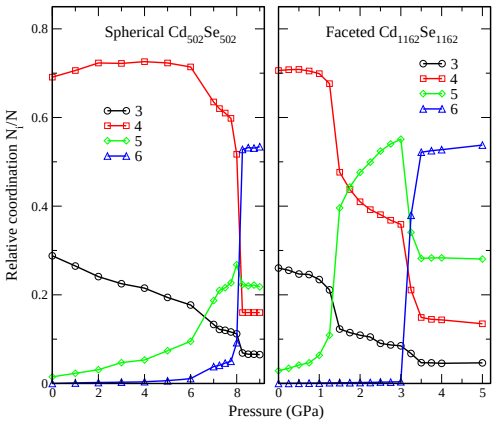


Wurtzite

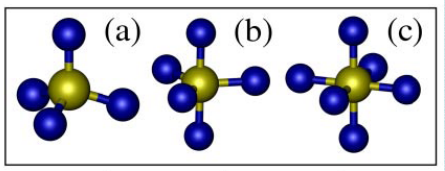
Apply Pressure



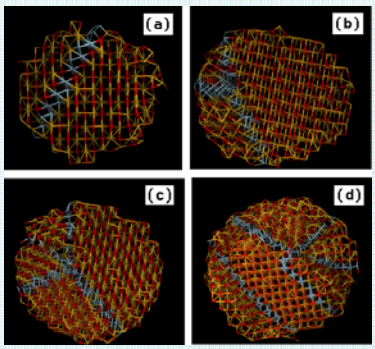
Rocksalt



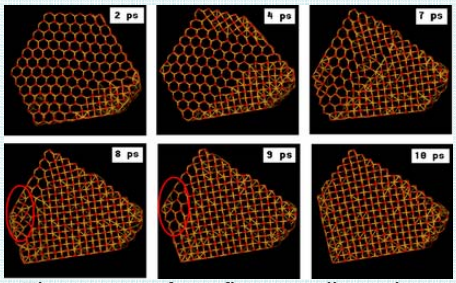
Coordination vs. Pressure



A five coordinated structure between wurtzite and rocksalt for faceted nanocrystal



Grain boundary for spherical nanocrystal



The process from five-coordinated to rocksalt for faceted nanocrystal

Conclusion

In summary by using the constant-pressure molecular dynamics method specially developed for finite system, the structural transformation of CdSe nanocrystals under hydrostatic pressure is studied. We have found the structural transformation of CdSe nanocrystal is highly affected by the size and shape. The results show that the critical pressure for WZ to RS structural transformation of spherical nanocrystal decreases with nanocrystal size, while it seems to increase for facet ones. For all spherical nanocrystals, the final structures have nano scale grain boundaries. All the faceted ones undergo uniform deformation, the transformed RS structure is of single domain nanocrystal.

Reference

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3) D. Y. Sun and X. G. Gong, J. Phys.: Condens. Matter **14**, L487 (2002).

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