Solution Structure from Small Angle X-ray Scattering of Surface Functionalized Polyethylene Imines II

B. Angelov[1], U. Vainio[2], A. Feoktystov[1], Y. He[3], and R. Willumeit[1]

[1]Institute of Materials Research, GKSS Forschungszentrum, Max-Planck-Str. 1, 21502 Geesthacht, Germany

[2] HASYLAB c/o DESY, Notkestr. 85, 22603 Hamburg, Germany

[3]DWI an der RWTH Aachen e.V. und ITMC, RWTH Aachen, Pauwelsstr. 8, 52056 Aachen, Germany

The solution structure of a partially branched polyethylene imine (PEI) that has covalently anchored functional groups has been investigated by SAXS. The ratio of primary, secondary and tertiary amine groups of the branched PEI was 31:39:30. It was synthesised from a commercially available derivative via covalent functionalization with cationic and hydrophobic groups [1]. The investigated model polymers have antibacterial applications [1]. They are cationic and can induce pore formation in the bacterial membranes, leakage and cell death.

Our experiments were performed at beamline B1 of the DORIS III storage ring at the synchrotron radiation facility HASYLAB/DESY in Hamburg, Germany. The beam size was 1.0 mm × 1.0 mm on the sample. The measurements were carried out at a fixed energy of 12 KeV, corresponding to a wavelength λ = 1.03 Å. The scattered intensity was recorded with a two-dimensional (2D) gas detector, the area of which was divided in 256 × 256 pixels. The SAXS data were averaged over the azimuth angle, normalized, background corrected, and calibrated.

The X-ray scattering pattern of 2 mg/ml functionalized PEI (synthesis described in ref.1) in aqueous solution was measured at room temperature (Fig.1). To obtain the corresponding atomic distance distribution function *p(r)*, we constructed a model. Our previous experience showed that programs like GNOM [2] and DAMMIN [3] do not reproduce realistically the structure of branched homopolymers. To make a more realistic PEI model, molecular dynamics [4] was used. On the basis of this model, the distance distribution *p(r)* was calculated directly as a sum of all inter atomic distances of the model molecule. The maximum diameter of the macromolecule was determined to be *70* Å. Since the branched PEI does not have a unique structure in solution, the presented model should be considered as an "equivalent" structure that reproduces the measured scattering curve. The structural studies will be extended to different stereo-chemical modifications of PEI in future.

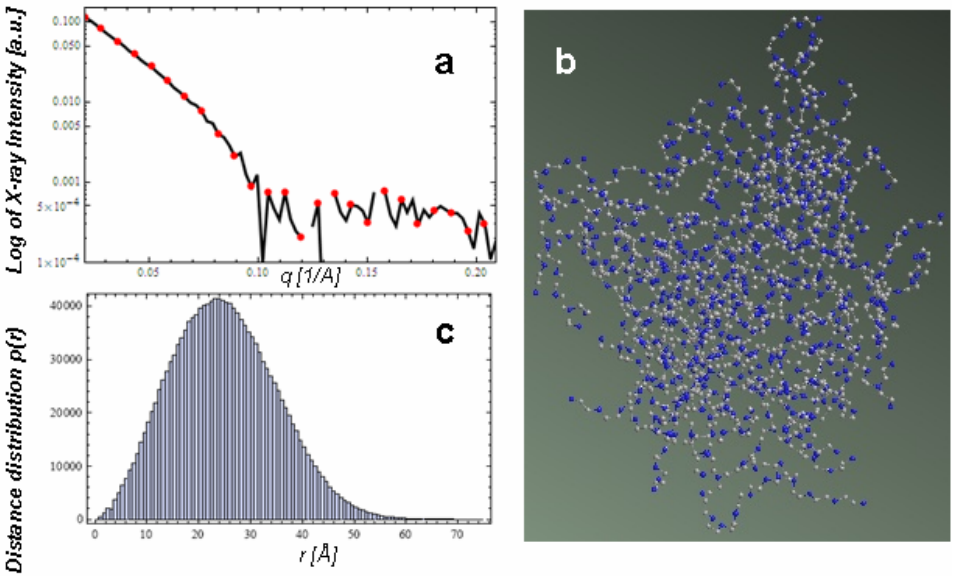

Figure 1: Example of measured X-ray scattering intensity of surface functionalized polyethylene imine (a), a model of the polymer structure (b), and the corresponding p(r) distance distribution function (c).

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References:

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