Fractal Geometry Applied To Fracture (Part 3)

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Glass Tutorial Series: prepared for and produced by the
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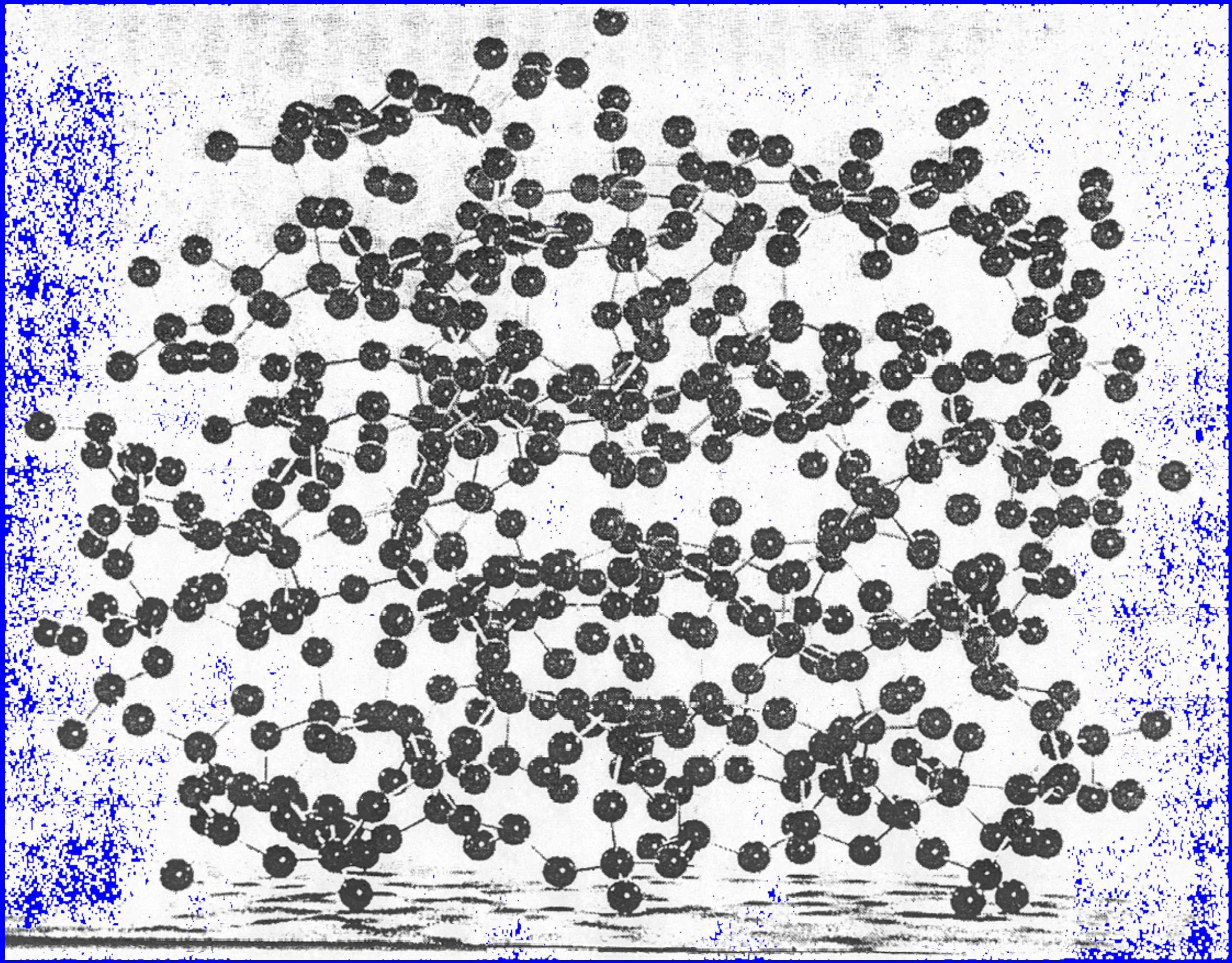
Technical Approach

- Molecular Orbital (MO) Modeling of Fracture - determines a_0.

- Molecular Dynamics (MD) Modeling of Fracture - determines D* (e.g. in Si)

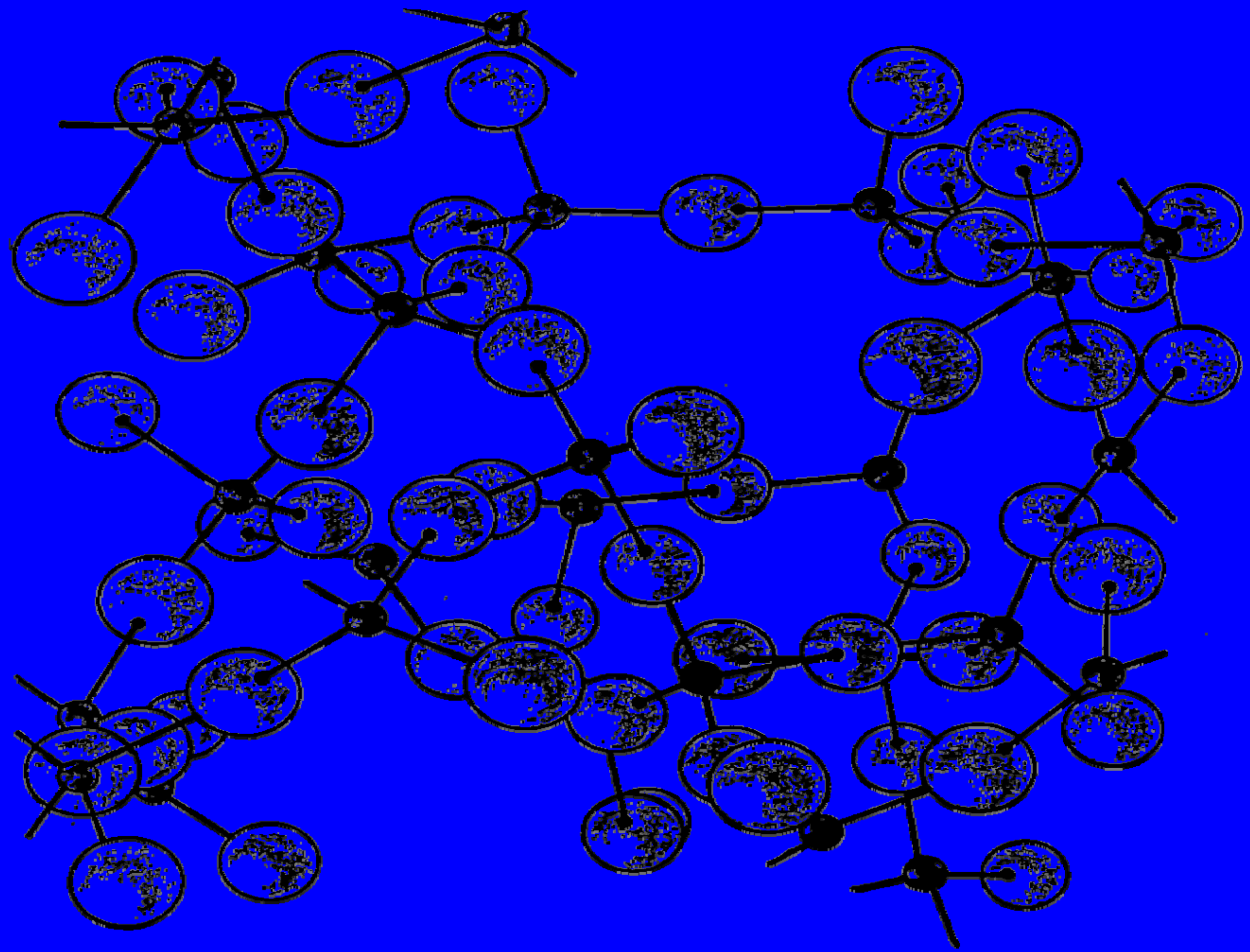
- Experimental determination and comparison of parameters obtained in MO and MD Modeling, i.e., a_0 and D*

Bell & Dean Model Used for MO Calculations

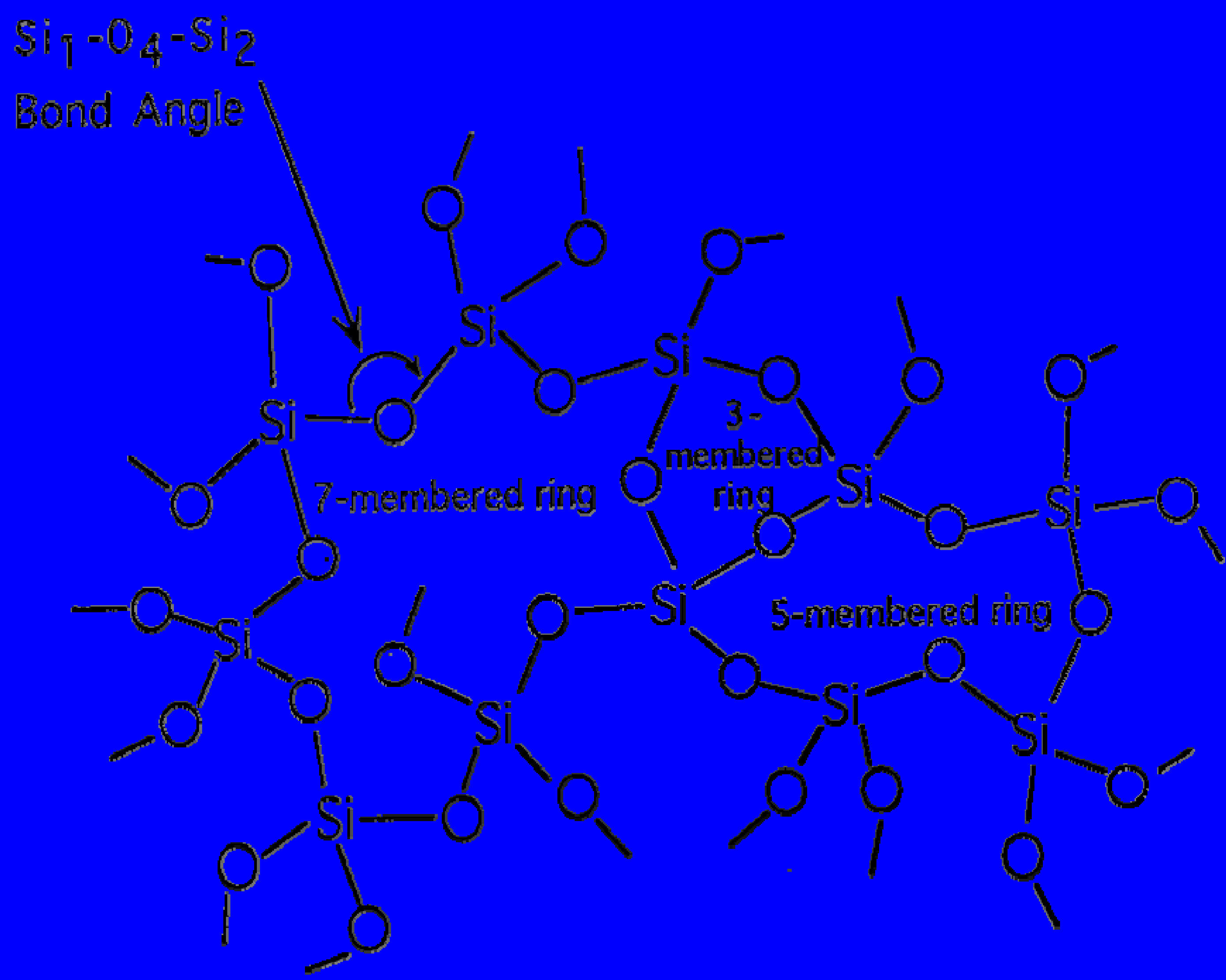


cf. Varsheneya, Fundamentals of Inorganic Glasses

(After Bell and Dean, Nature 212, 1354 [1966])

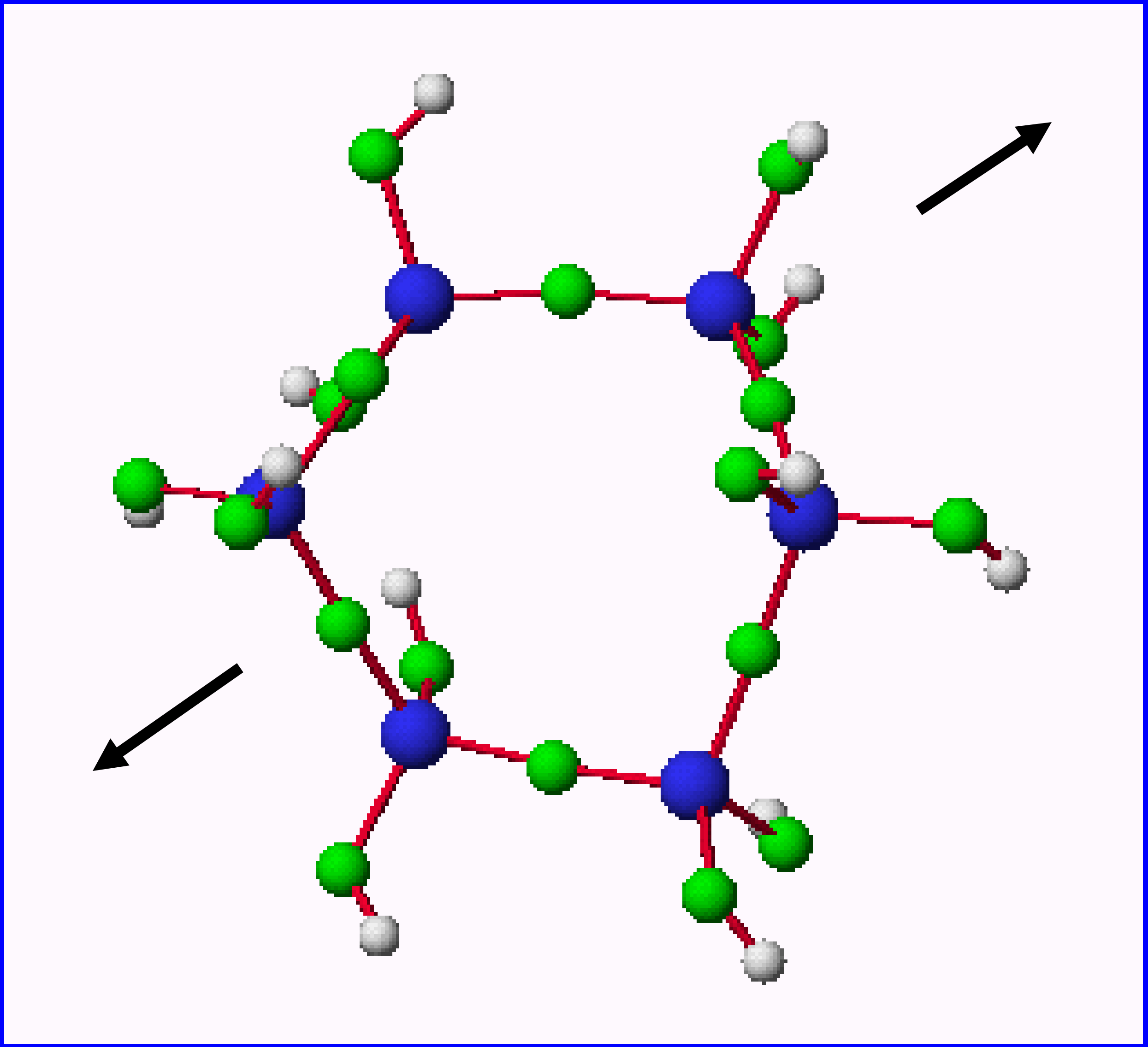


cf. Varsheneya, Fundamentals of Inorganic Glasses
(after T. F. Soules, Glass Sci & Tech 4A, 318)

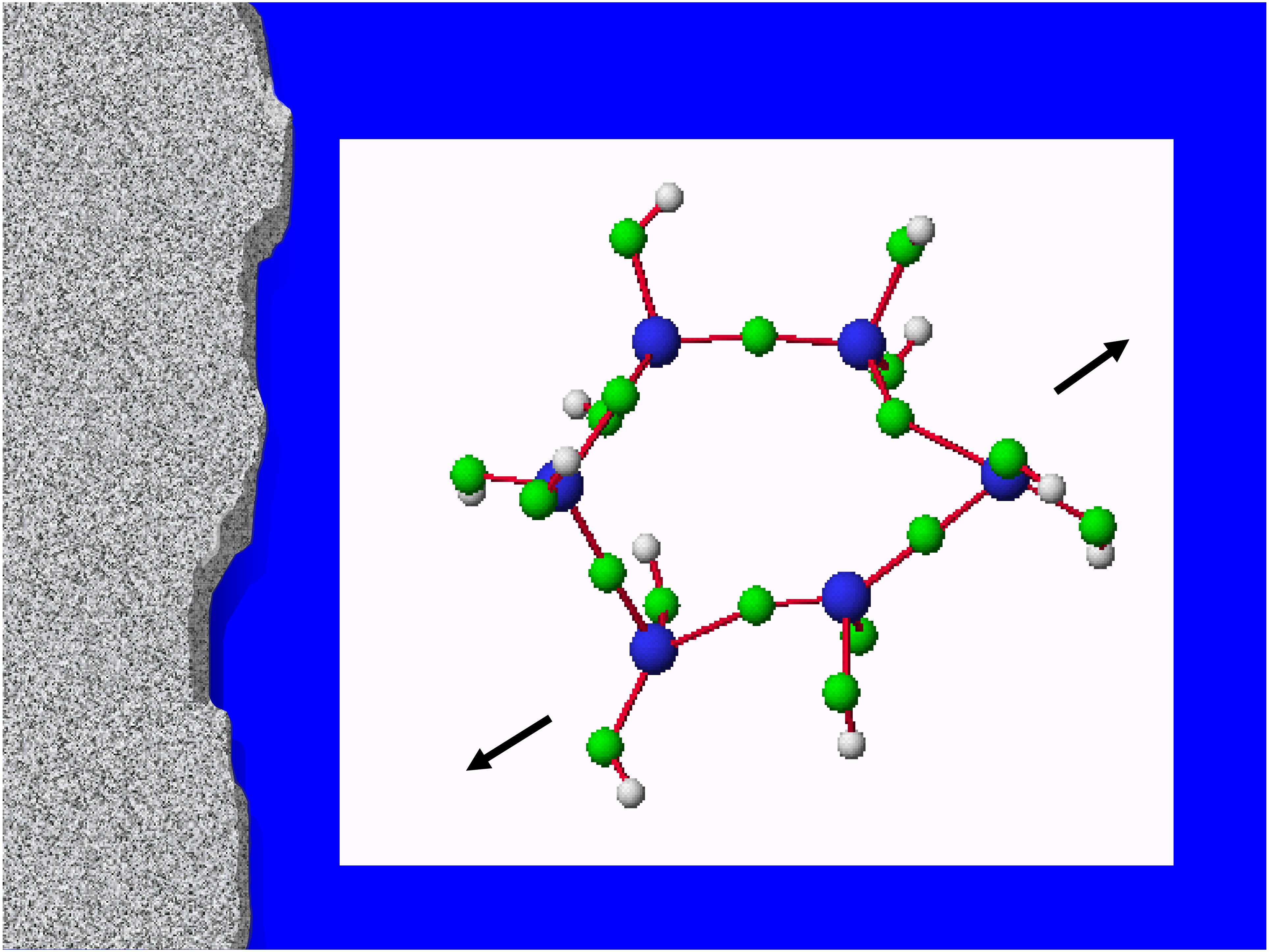


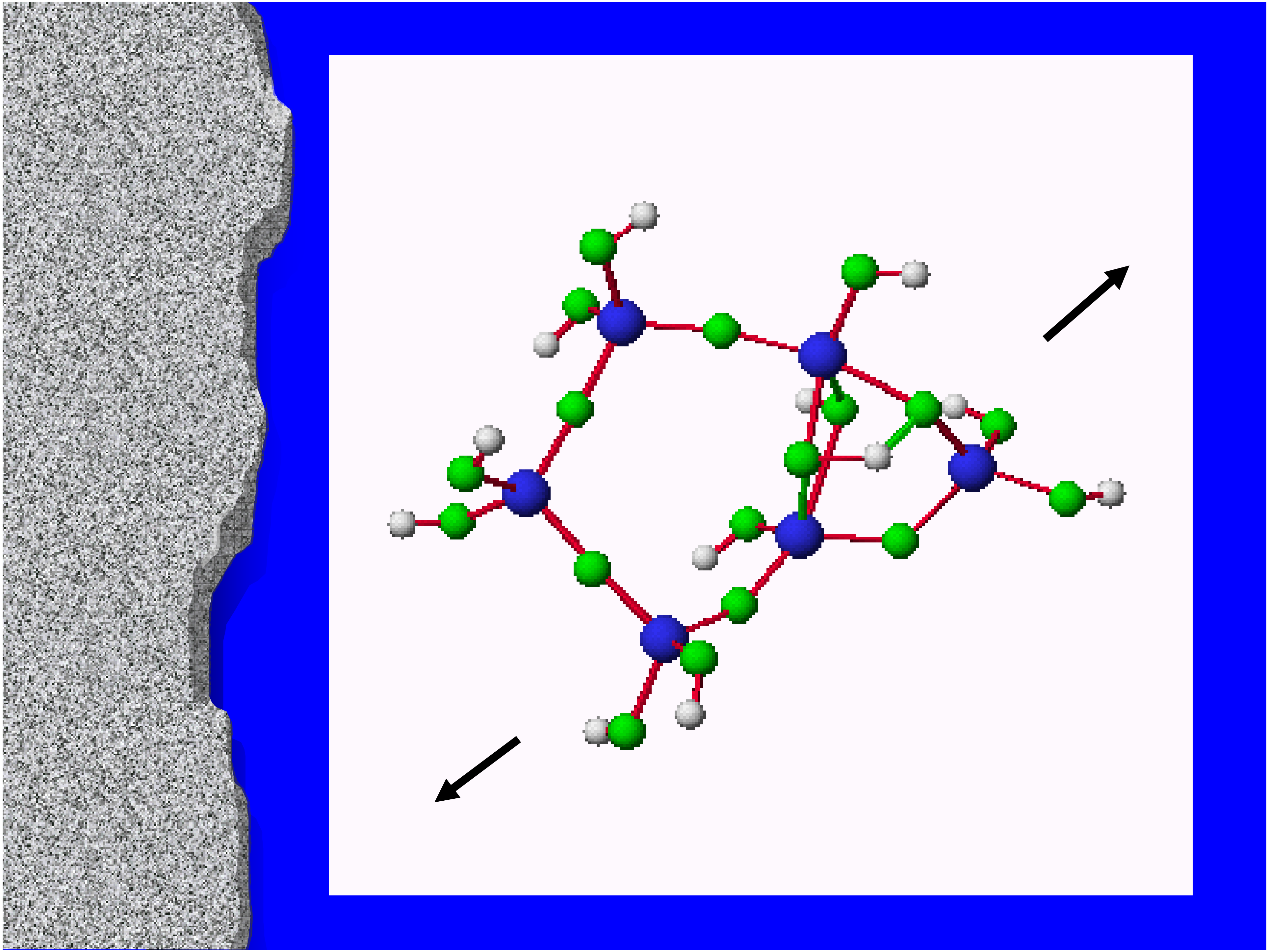
cf. Varsheneya, Fundamentals of Inorganic Glasses

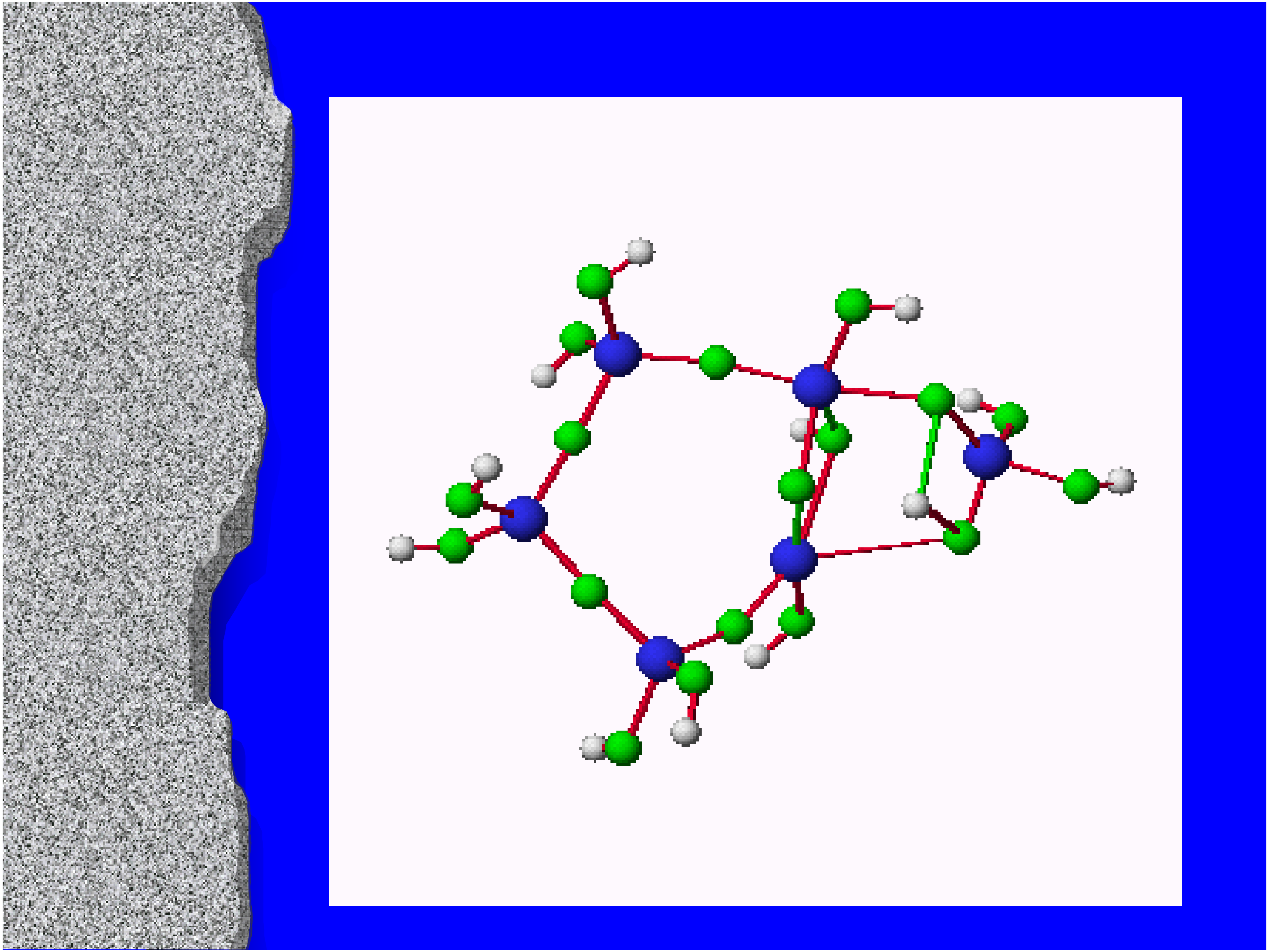
MO Simulates Bond Breaking At The Crack Tip

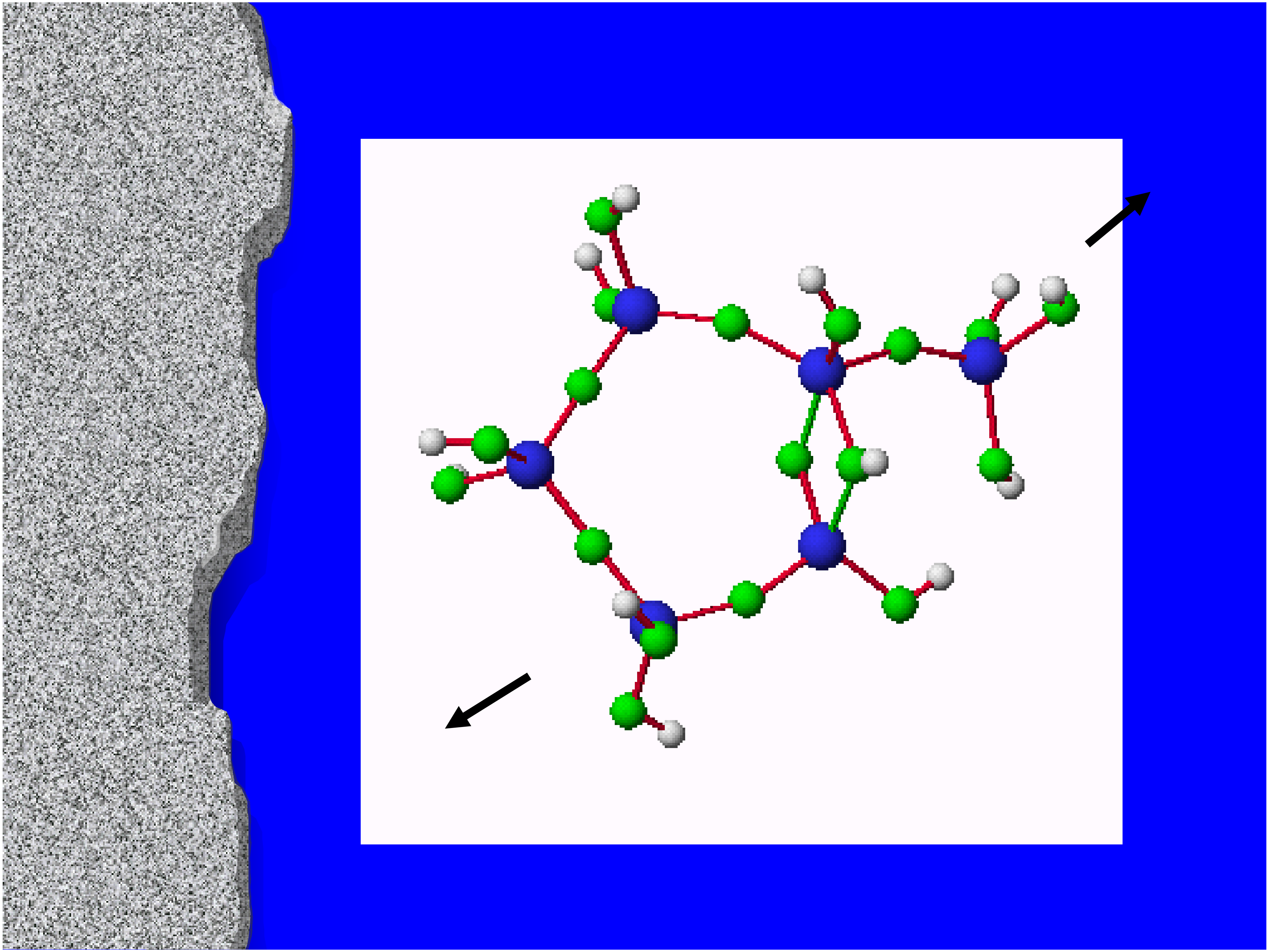


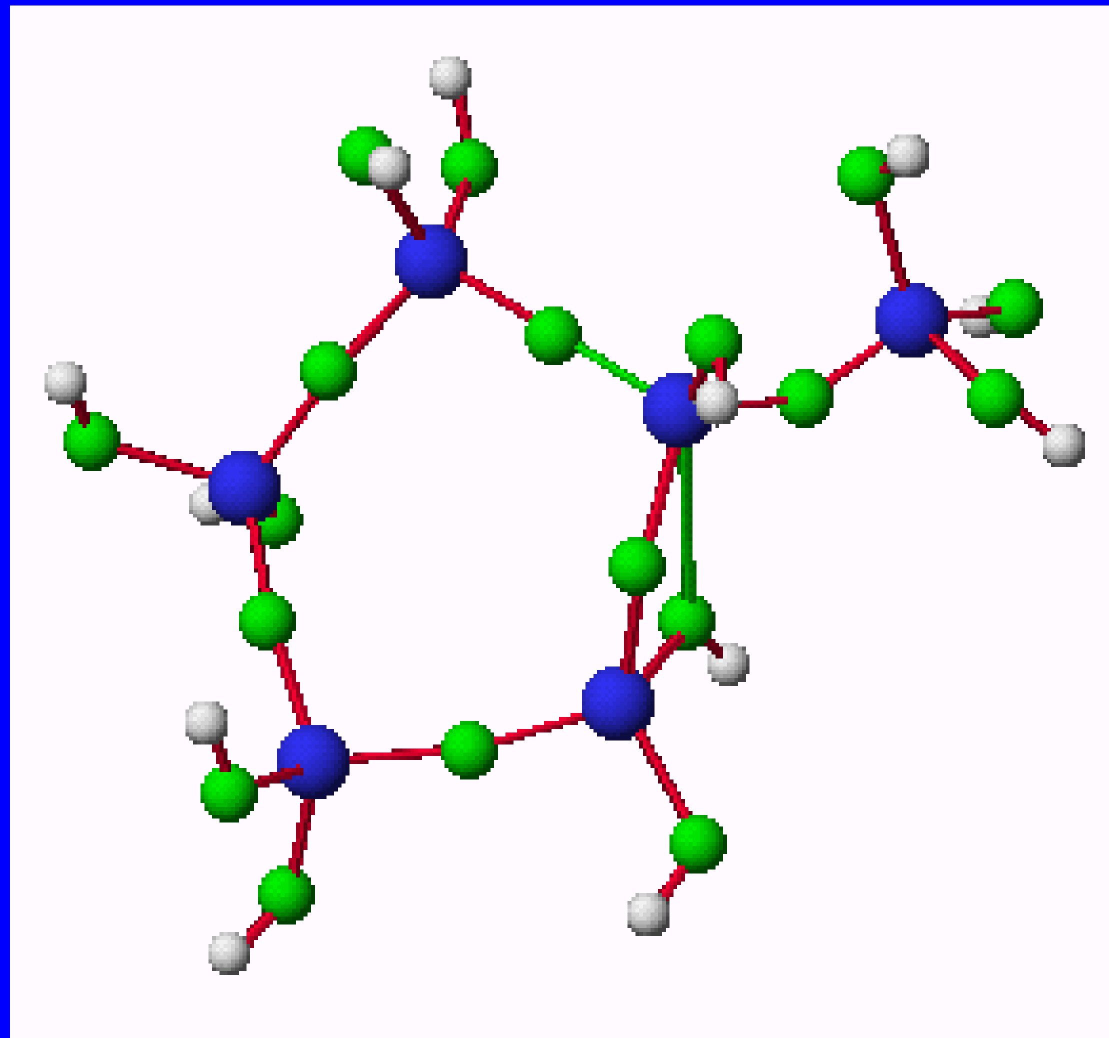
Simulated SiO_2 Δ displ.= 1 Å

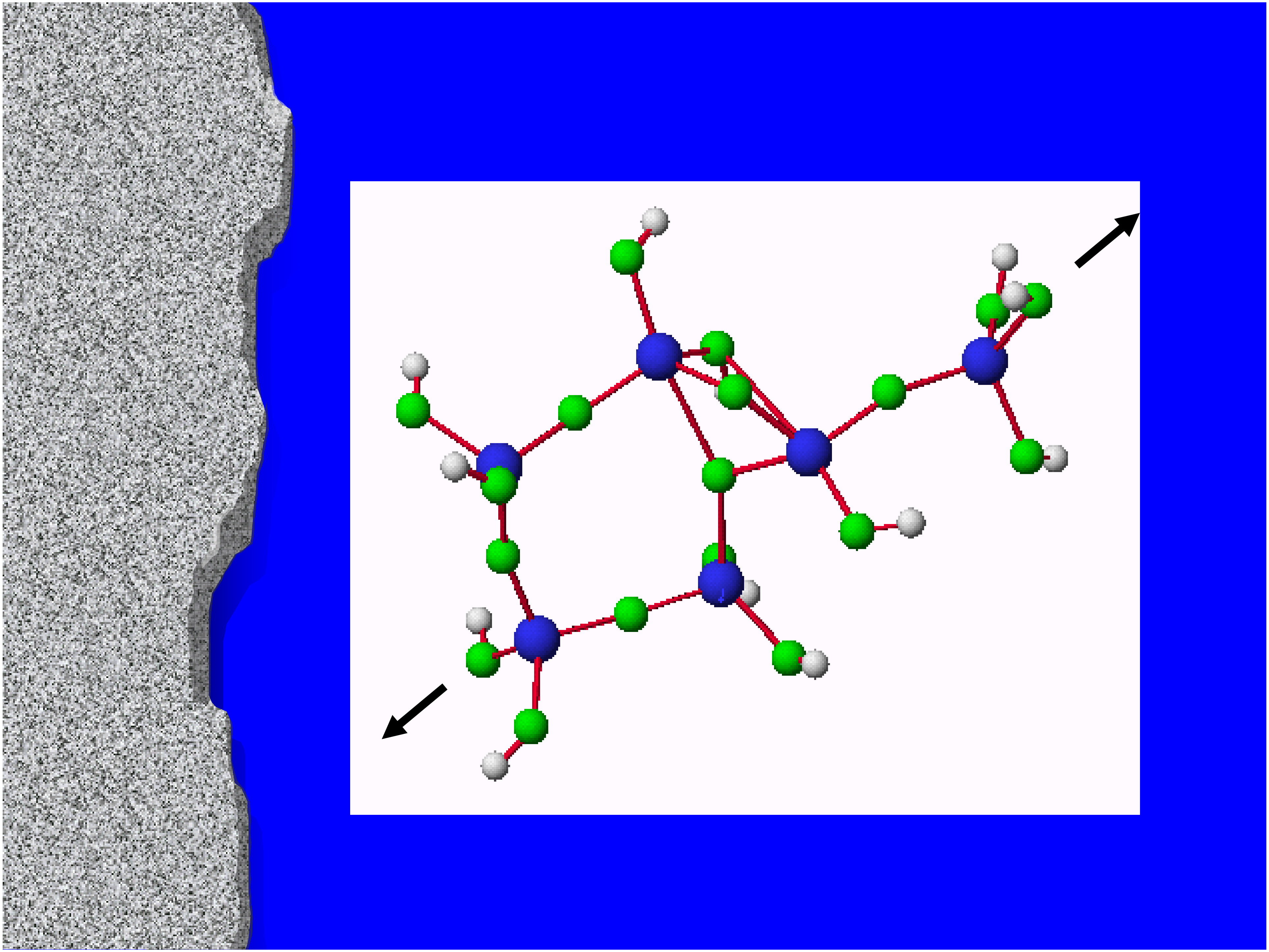


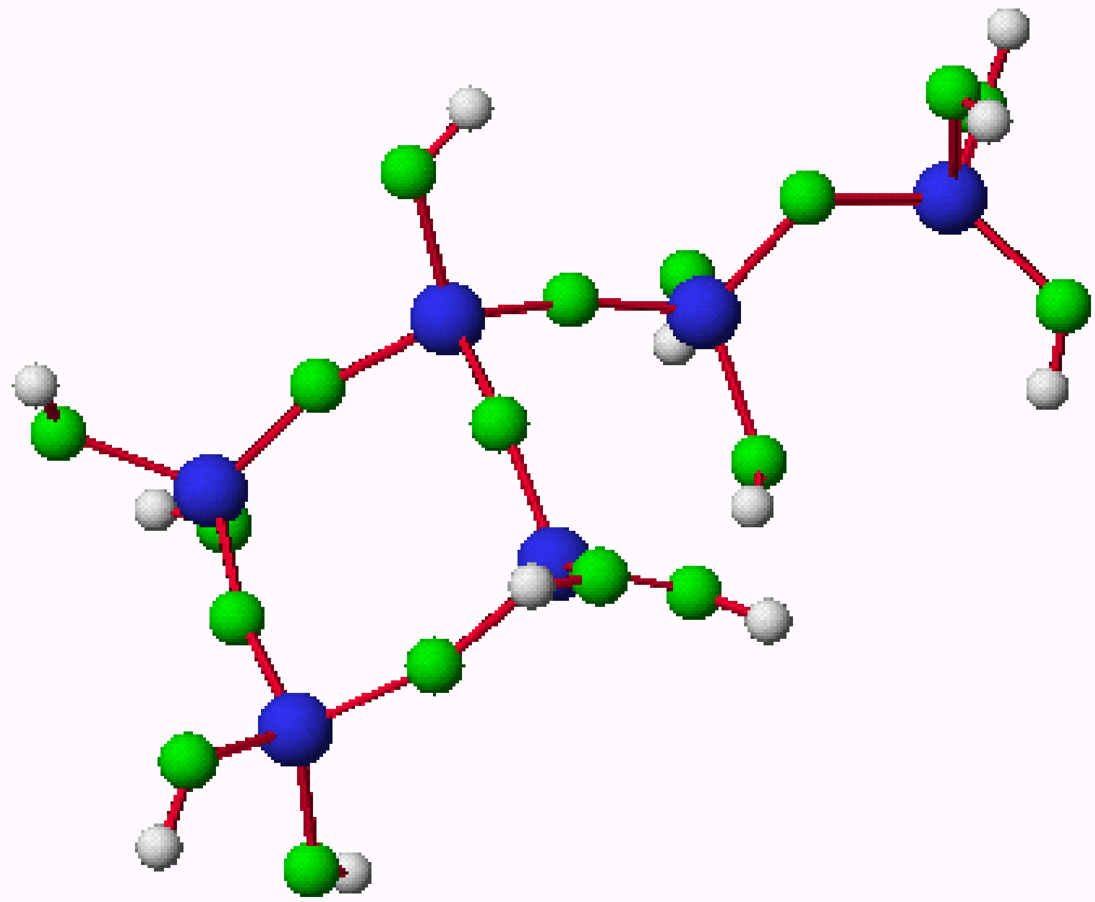


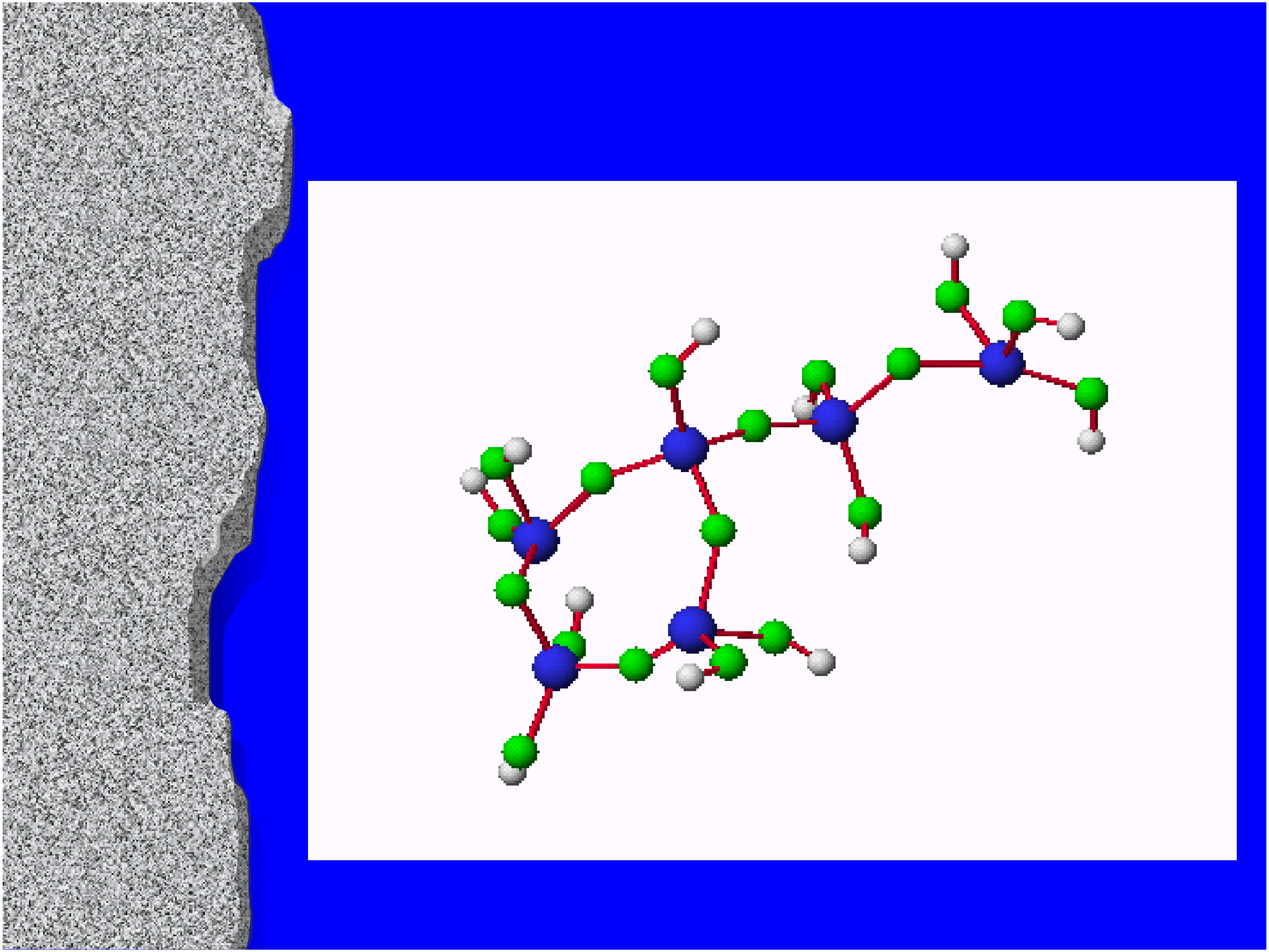


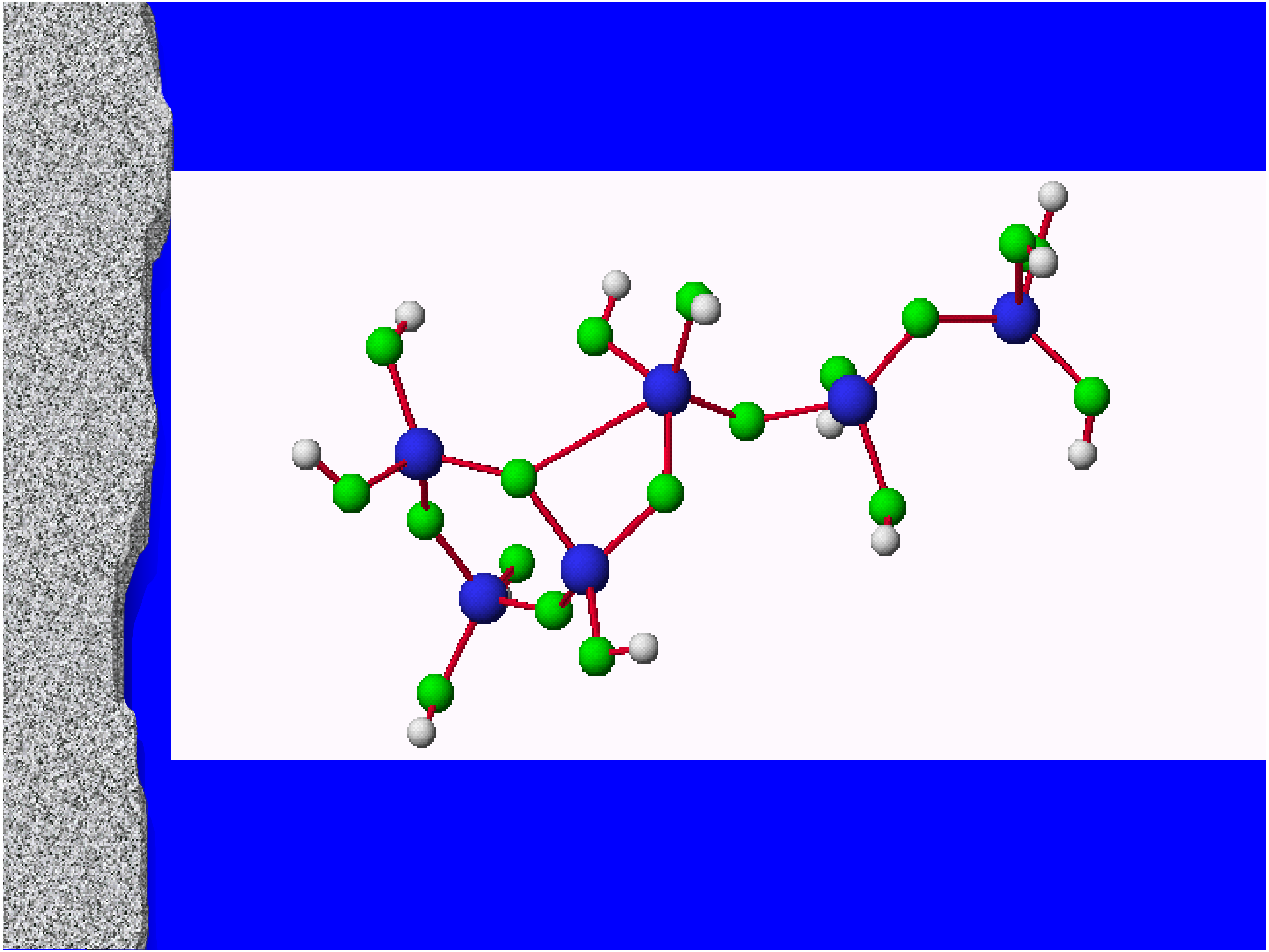


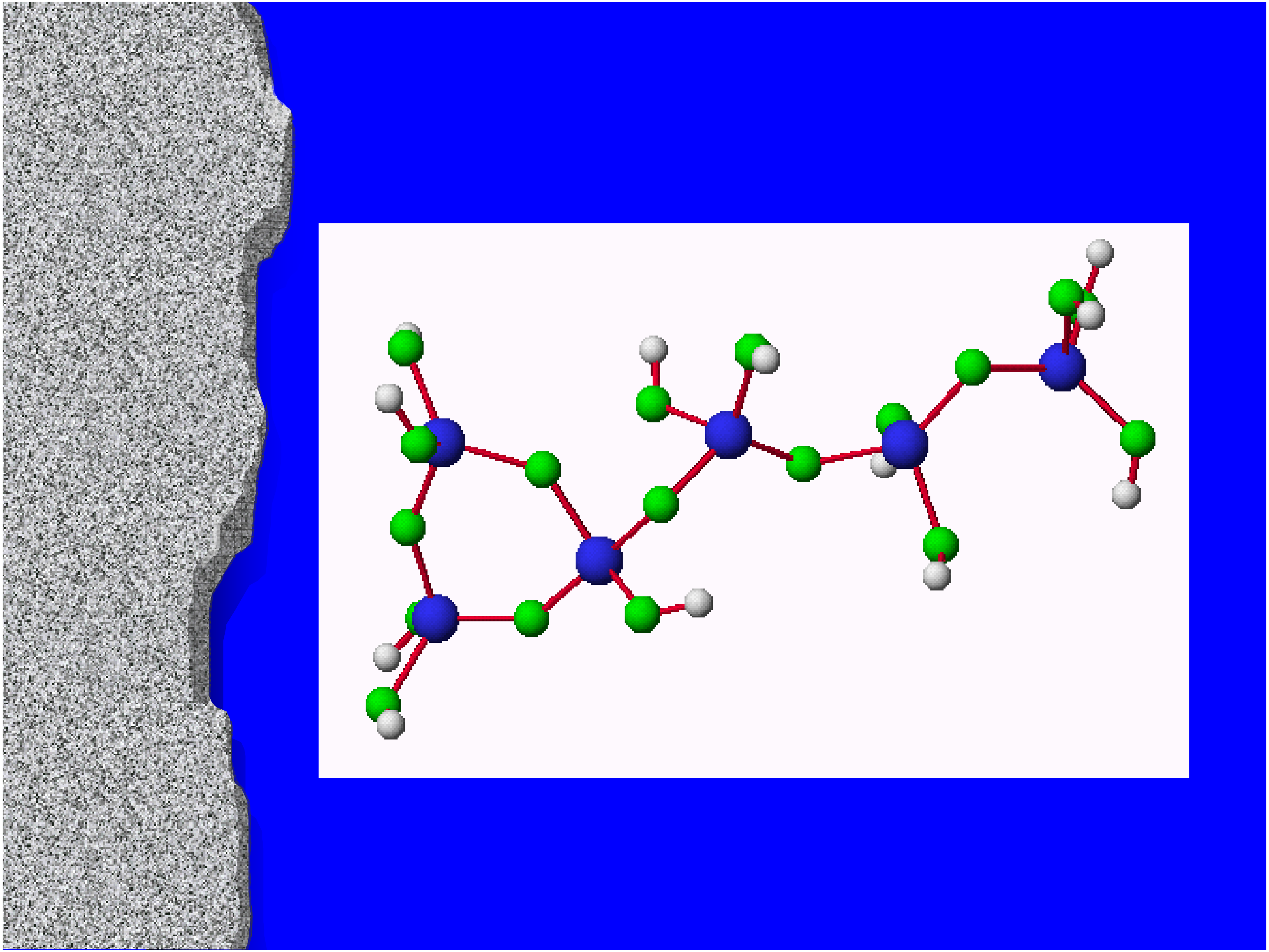




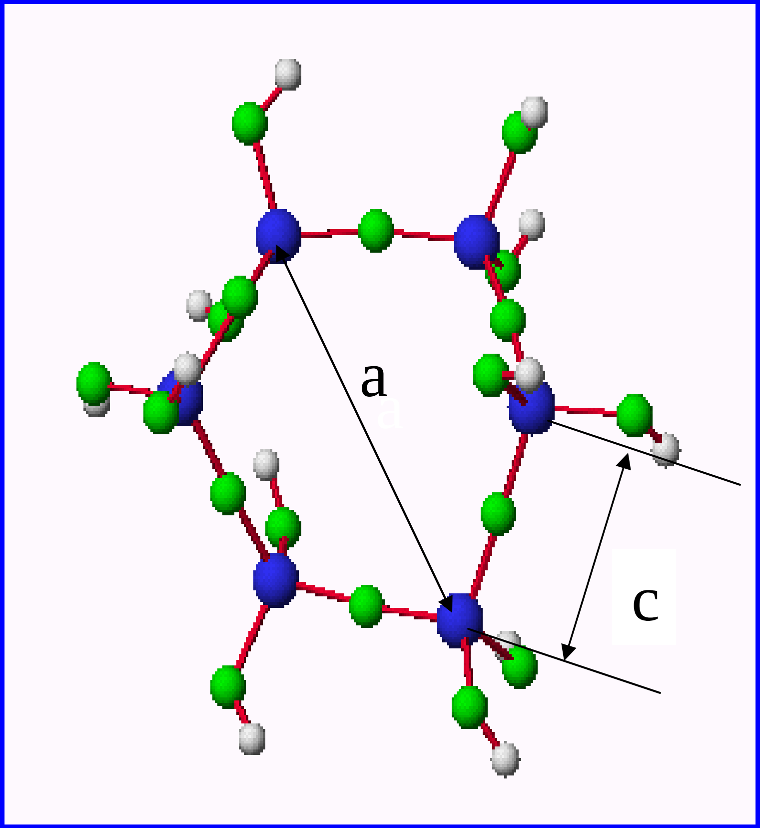








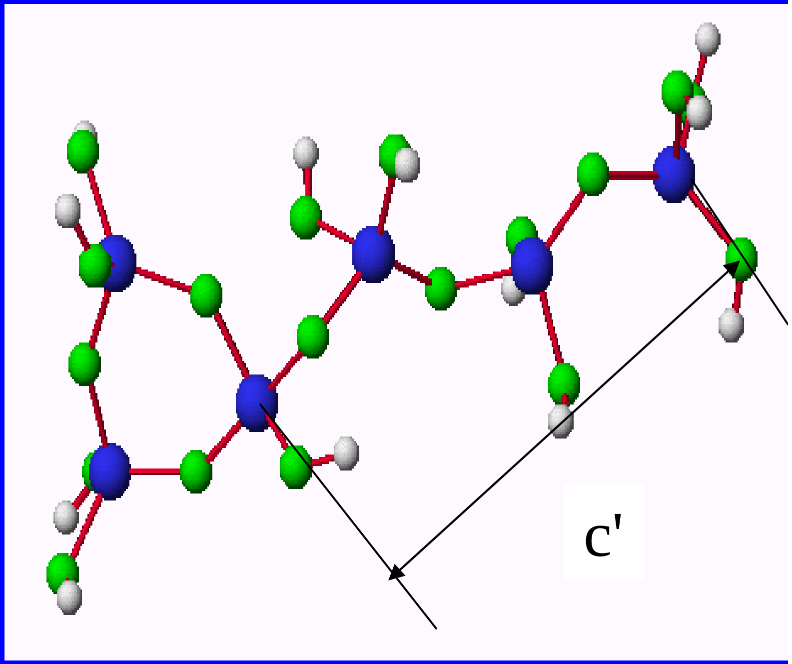
Strain Can Be Measured In Model



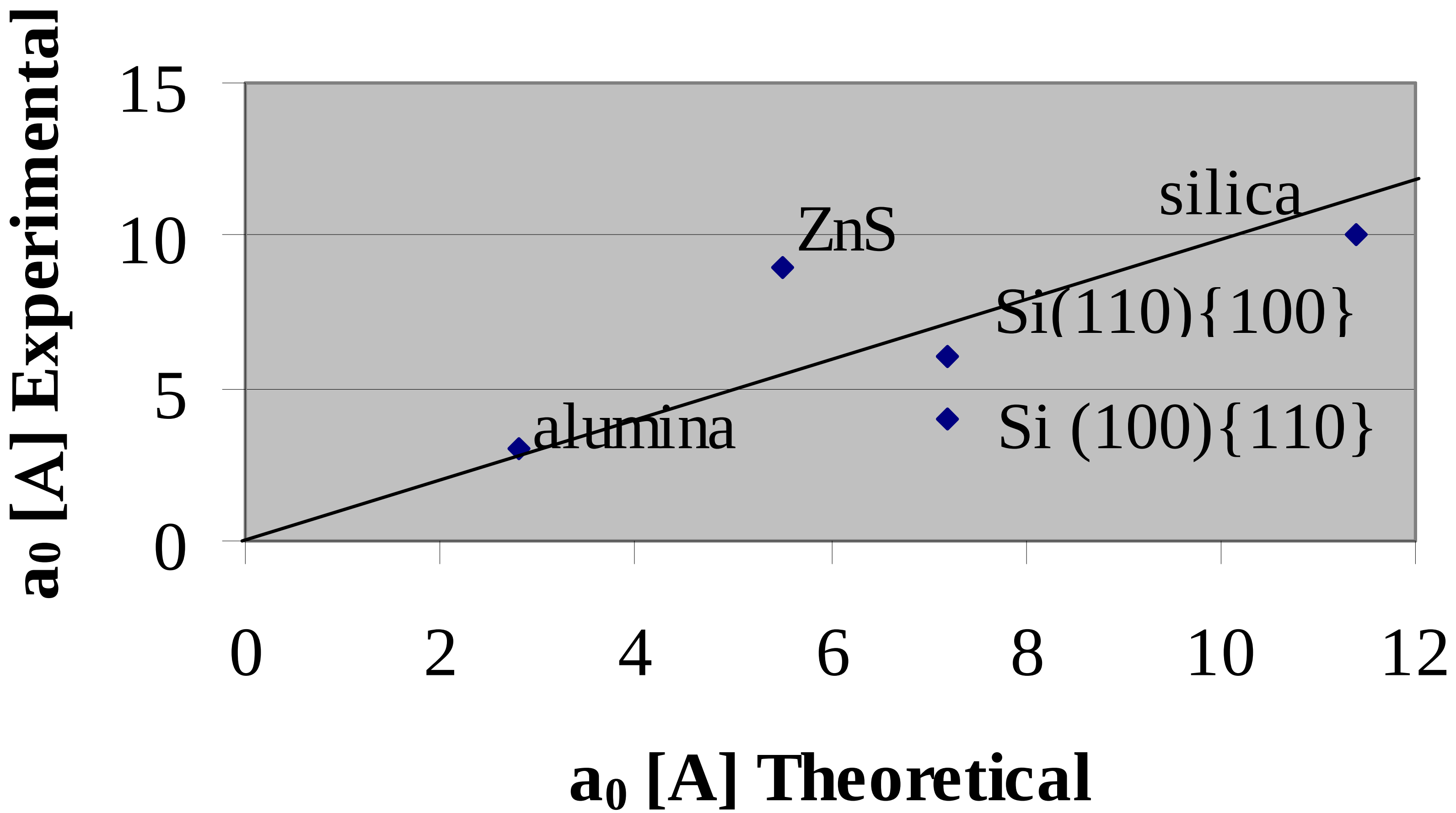
J. Non-Crystalline Solids 260 (1999) 99-108.

$$a_0 = a / \varepsilon$$

$$= c\, a / c' - c$$



Modeling and Experimental Results Agree



$a_0 = 2\gamma / (ED^*)$

J. K. West, J. J. Mecholsky, Jr, and L. L. Hench, "The Quantum and Fractal Geometry of Brittle Fracture", J. Non-Crystalline Solids 260 (1999) 99-108.

a_0 Is Related To Structure

Material Class		a_0 (Å)
Single Crystals		1-10
Glasses		10-20
Glass Ceramics		20-80
Polycrystalline Ceramics		3-10
Polymers		2700-14000

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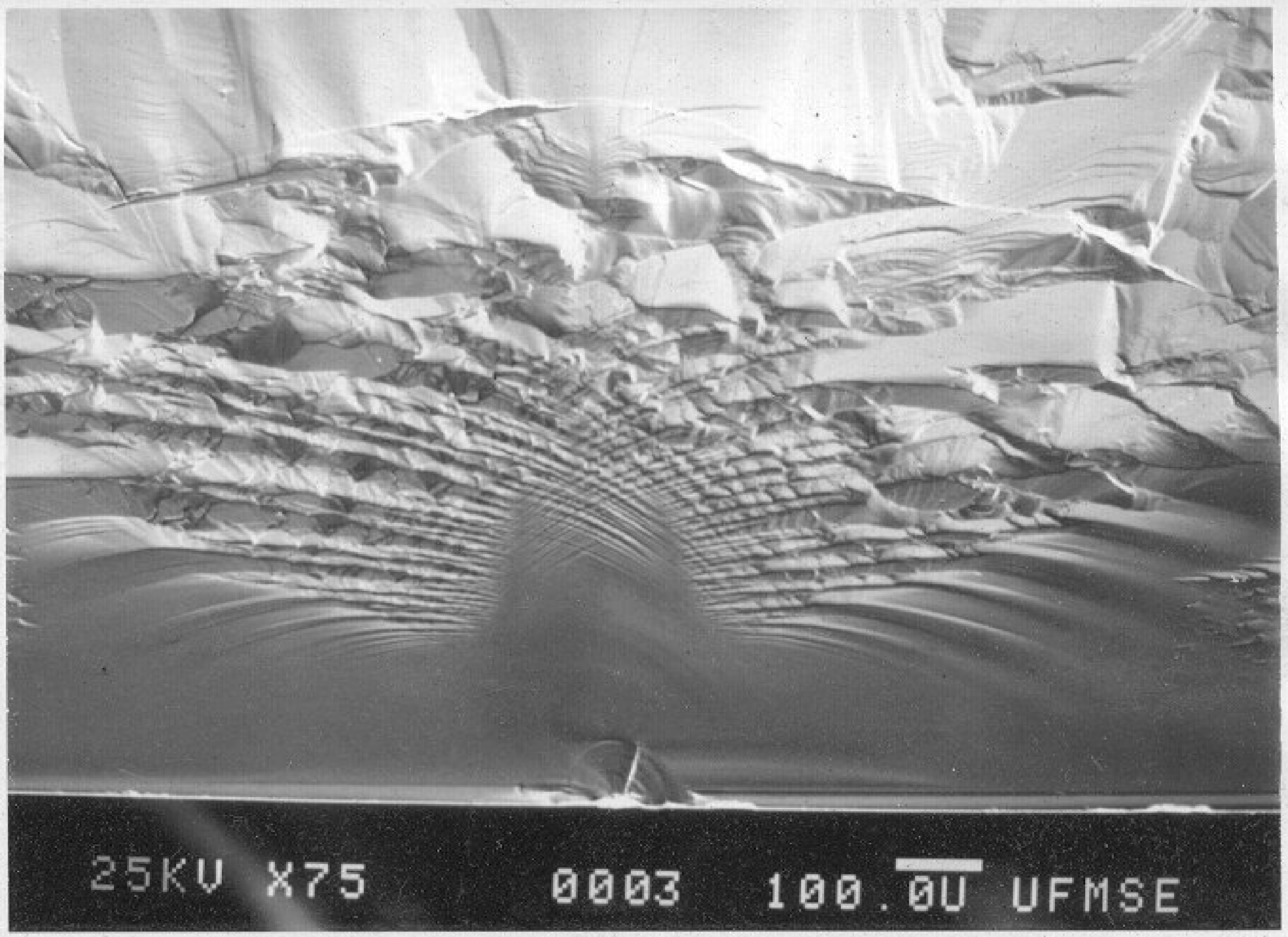
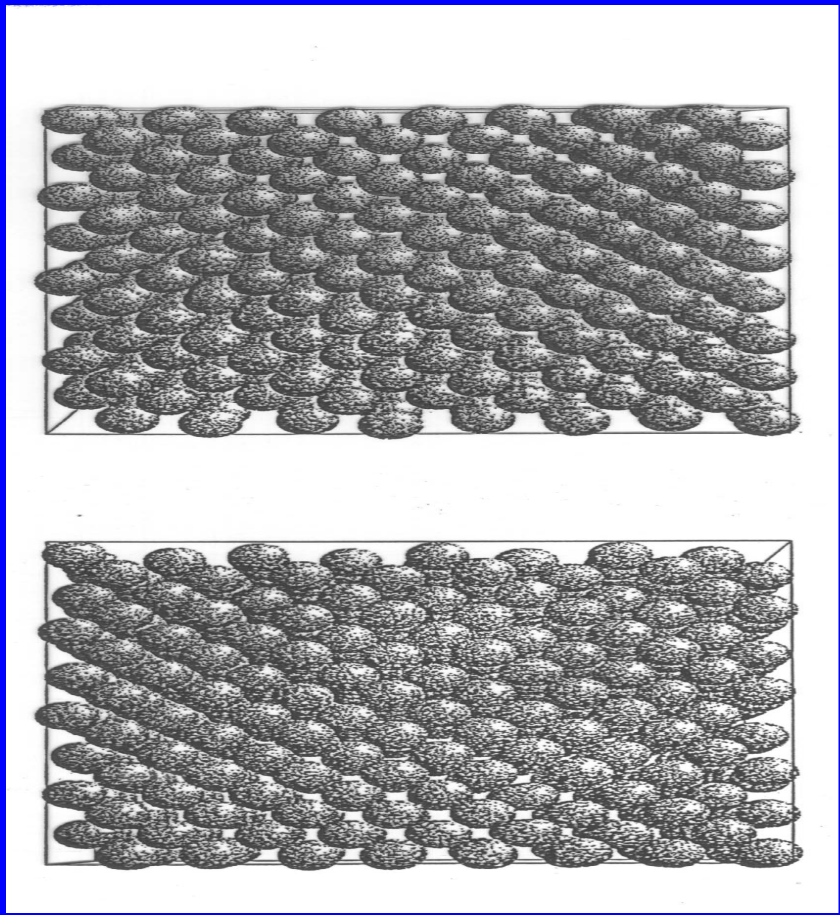
FSA Can Be Applied To Single Crystals

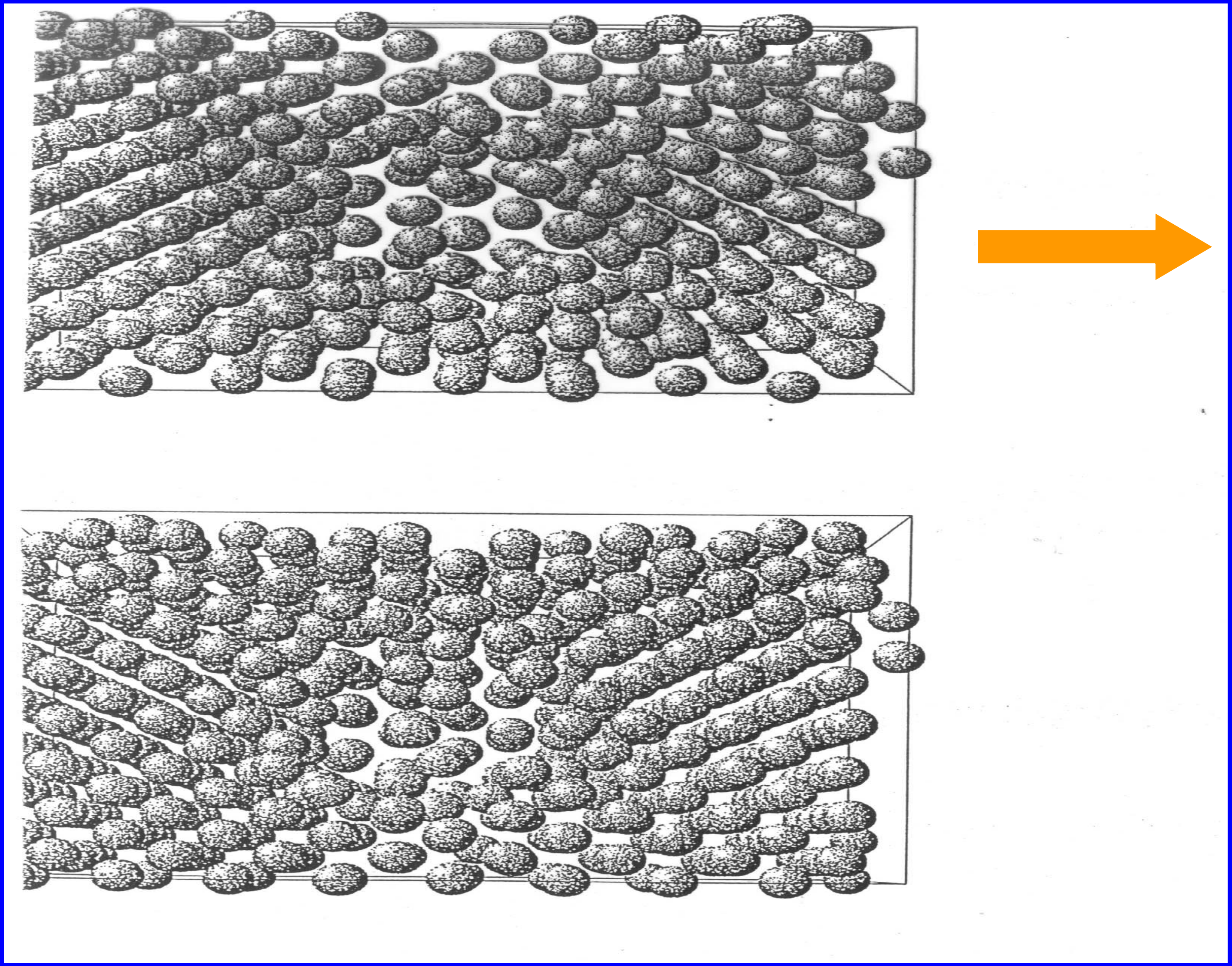


Single Crystal Silicon

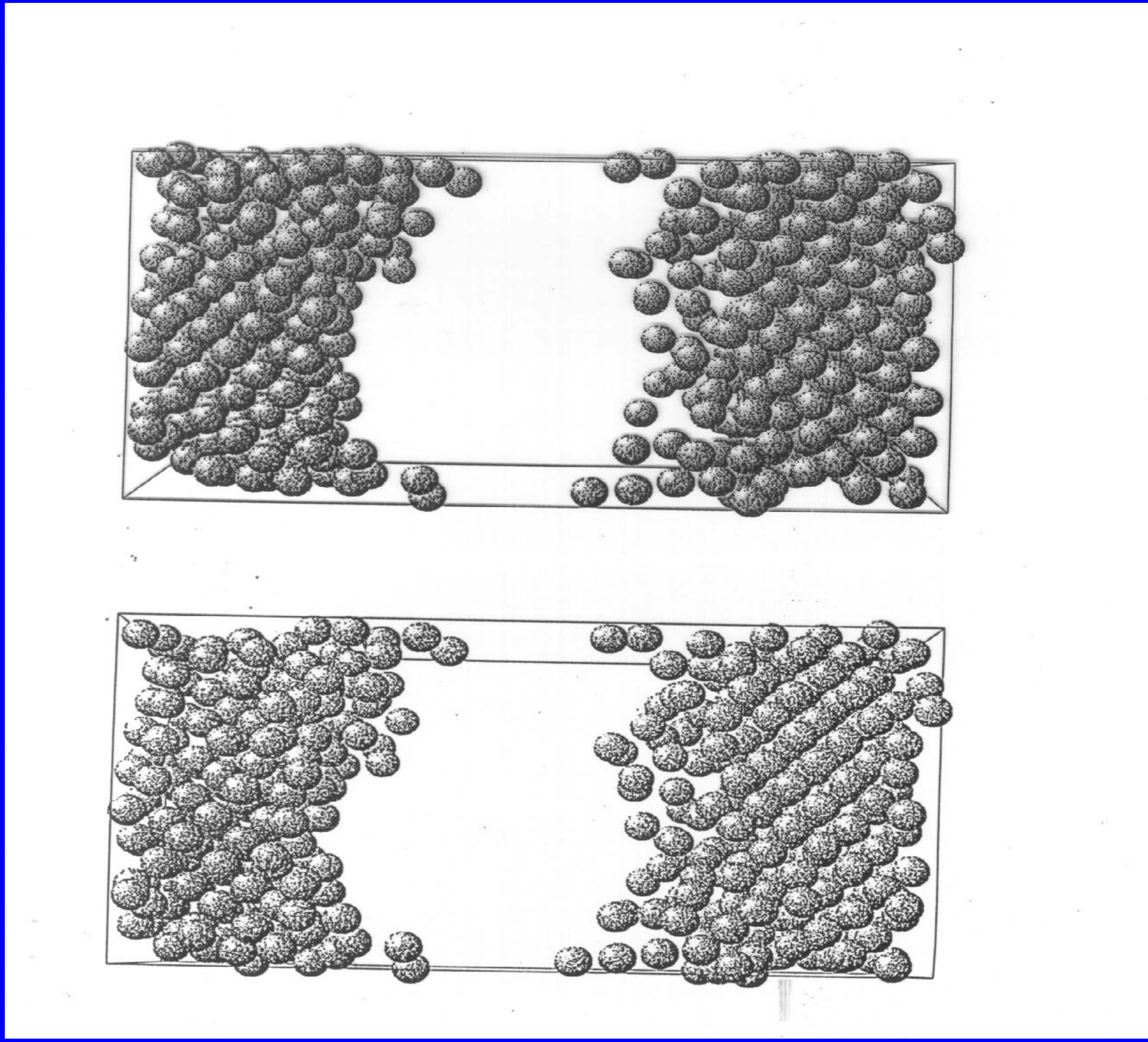
Simulated Fracture Can Form Fracture Surface



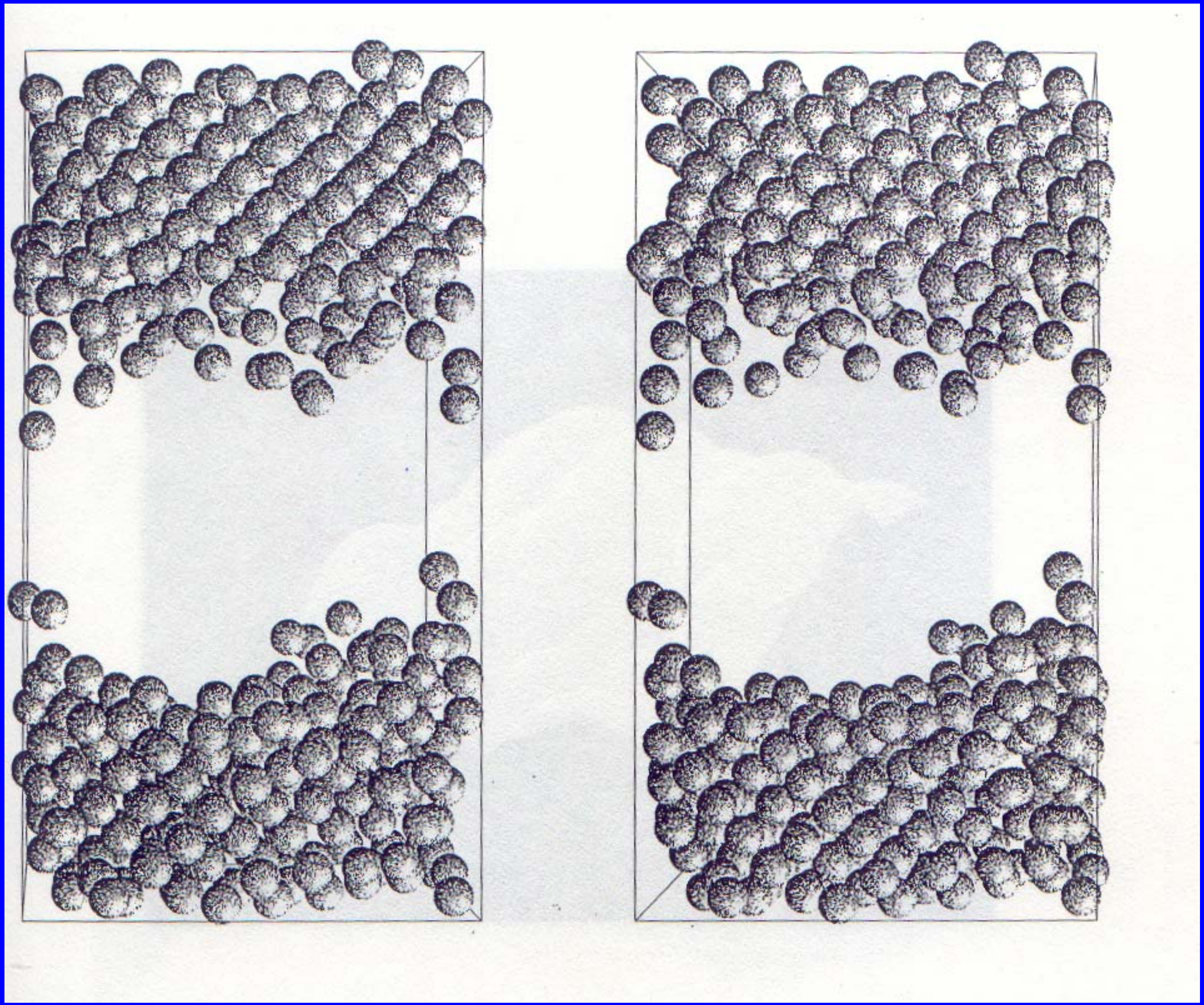
Simulated Fracture Can Form Fracture Surface



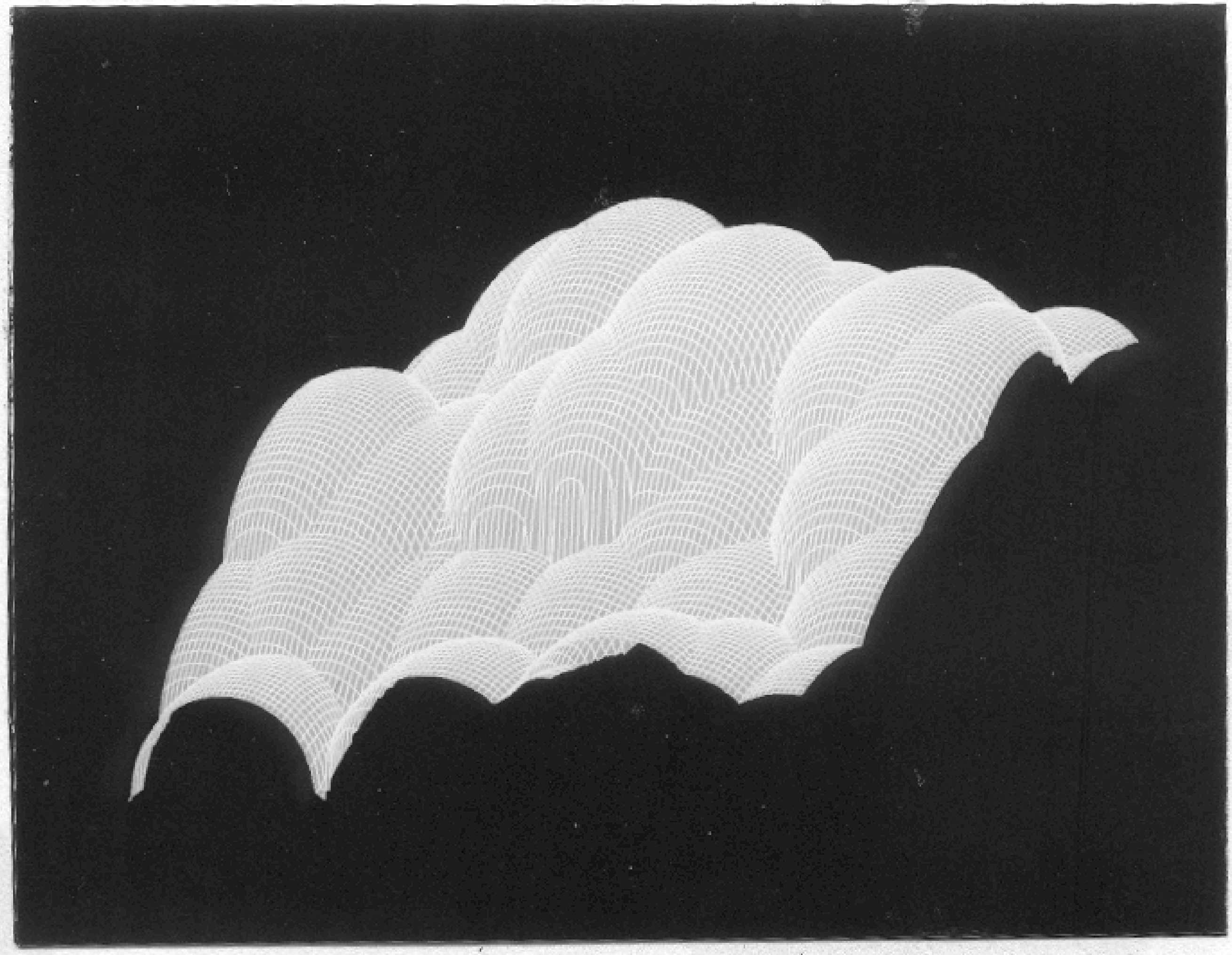
Simulated Fracture Can Form Fracture Surface



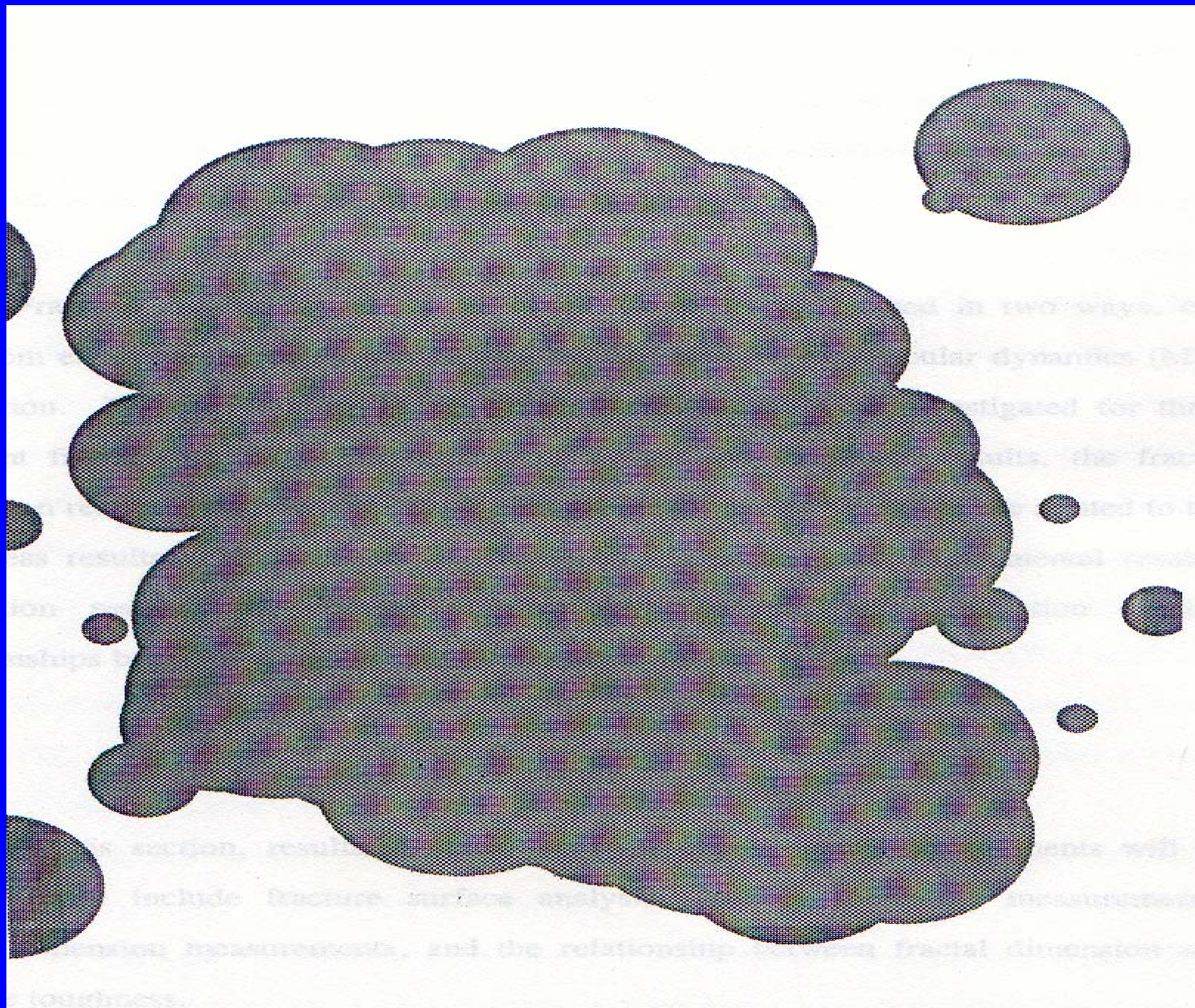
Simulated Fracture Can Form Fracture Surface



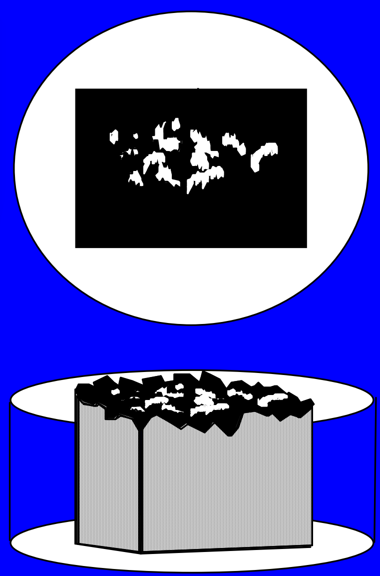
Surface Can Be Created From MD Simulation

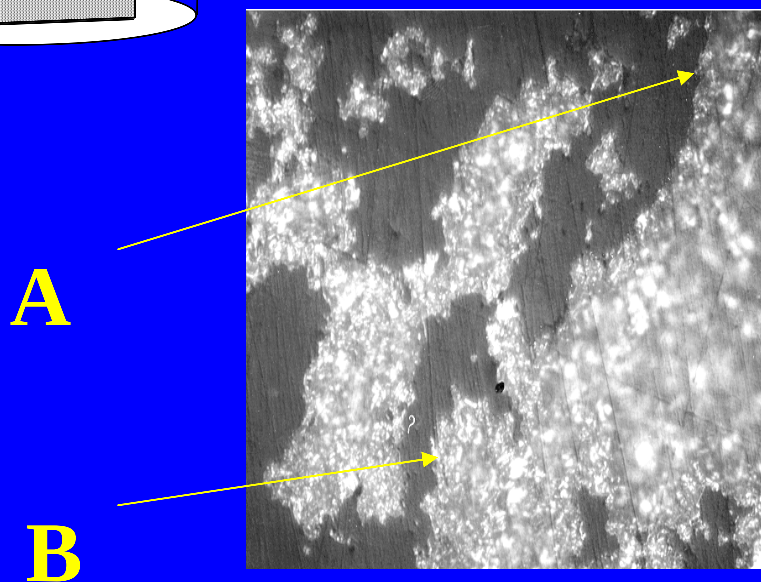


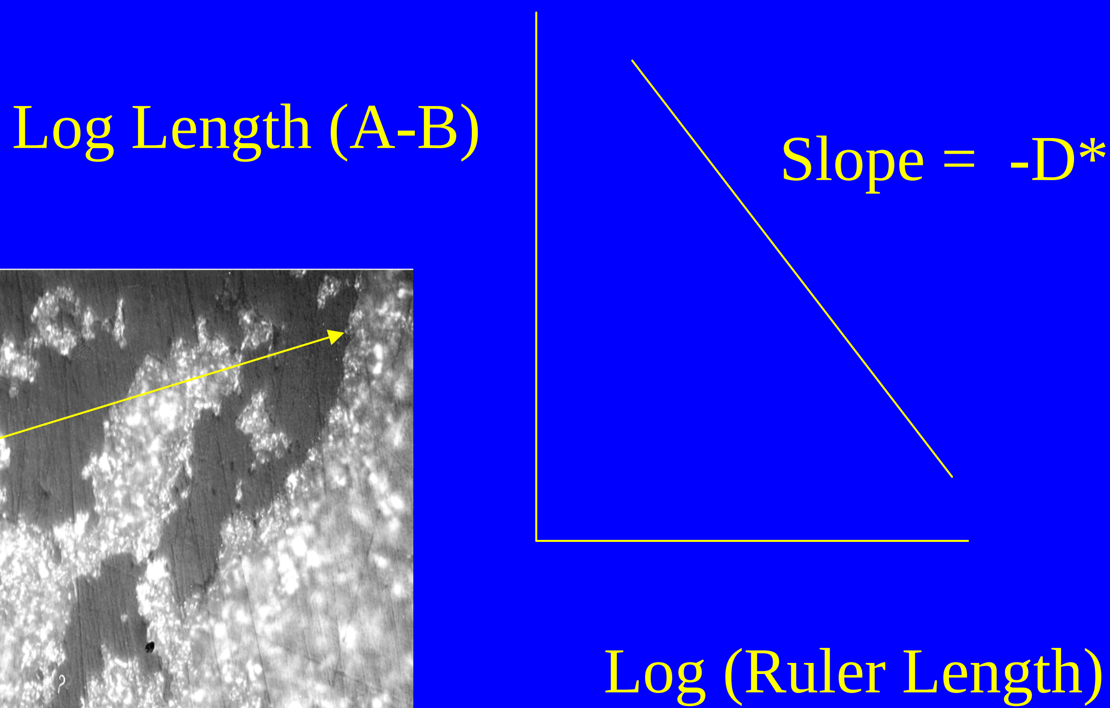
Slit Island Contour Can Be Made From 3-D Map



FRACTAL DIMENSION IS MEASURED ALONG CONTOUR





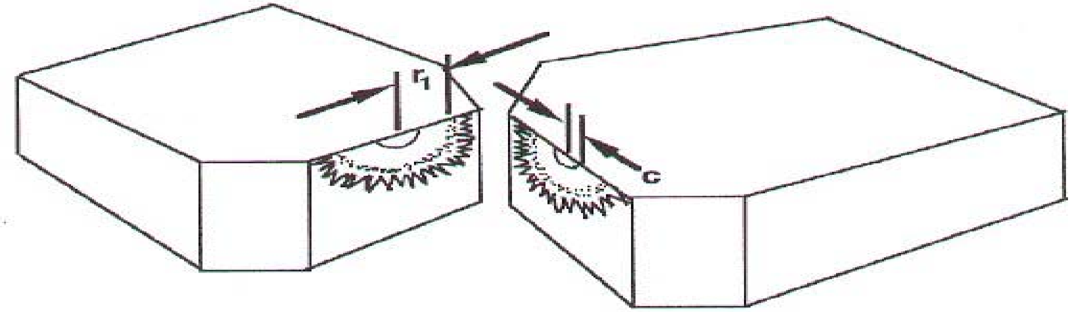


A-B = Slit Island Contour

MD Simulations & Experimental Results Agree

Material Fracture Plane/Surface	K_{IC} (MPam$^{1/2}$)	Fractal Dimension (Experimental)	Fractal Dimension (MD Simulation)
Si {100}/{110}	**1.26 ± 0.06**	**2.16 ± 0.04**	**2.16 ± 0.06**
Si {110}/{100}	**1.23 ± 0.08**	**2.10 ± 0.04**	**2.11 ± 0.05**
Si {111}/{110}	**1.17 ± 0.08**	**2.06 ± 0.02**	**2.09 ± 0.04**
Silica (amorphous)	**0.75**	**2.11± 0.02**	**2.1**

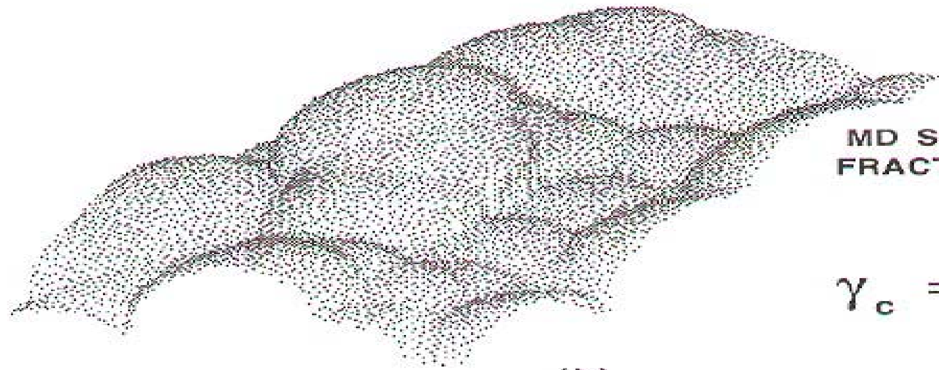
Y. L. Tsai, T. P. Swiler , J. H. Simmons and J. J. Mecholsky, Jr., in Computational Modelling of Materials and Processing, J. H. Simmons, et al. (eds) The Am. Cer. Society, Ceram. Trans. 69 (1997) 217.



CRACK SIZE (c) to MIRROR-MIST (r_1) RATIO: $D^* = \frac{c}{r_1}$

where D* = FRACTAL DIMENSIONAL INCREMENT

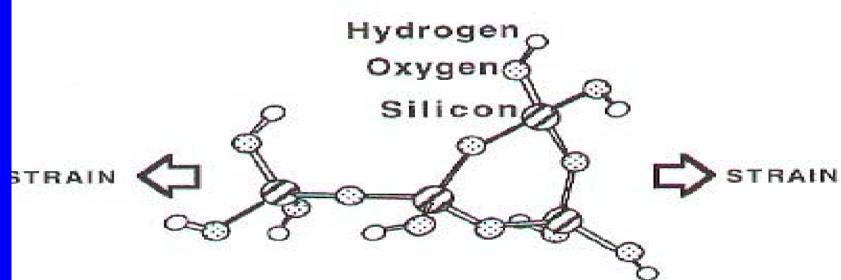
(a)



MD SIMULATION OF FRACTAL FRACTURE SURFACE

$$\gamma_c = \frac{a_o D^* E}{2}$$

(b)



AM1 MO MODEL OF FRACTURE AS ATOMIC LEVEL RING CONTRACTION

RING DIAMETER TO STRAIN FRACTION RATIO: $a_o = a/\varepsilon$

(c)

Fracture Is A Fractal Process

- Fracture transcends many length scales; Self-similar (or self-affine), scale invariant & characterized by D*.
- Hypothesis: $2\gamma = [a_0 E D^*]$
- Observations seem to support the hypothesis.

$$c/r = D^* \quad ; \quad \gamma \propto ED^*$$

(D* is a geometric & energy scaling factor.)

(a_0 is a fracture surface structural element)

- MD & MO modeling provide framework for understanding macroscopic observations

Many Tools Are Needed for Unified Fracture Theory

Model	Scale	Experiment
MO	sub-atomic	fractoemission
Ab initio	atomic	AFM
Quantum	nano	STM
Mechanics		Raman
		Fluorescence
MD	micro	crack velocity
Monte Carlo		SEM
Finite diff.	Meso	AFM
FEM	Macro	fractography
		fracture mechanics

Fractal Geometry

Fracture Process

Summary

- At the atomic level, quantum mechanics describes the fracture process as a ring contraction process dictated by minimum energy and availability of free volume.

- On the molecular scale, MD modeling describes creation of the fracture surface.

- On the macroscopic scale, mirror, mist & hackle form & c/r = D*

- At all length scales, $2\gamma = [a_0 \ E \ D^*]$

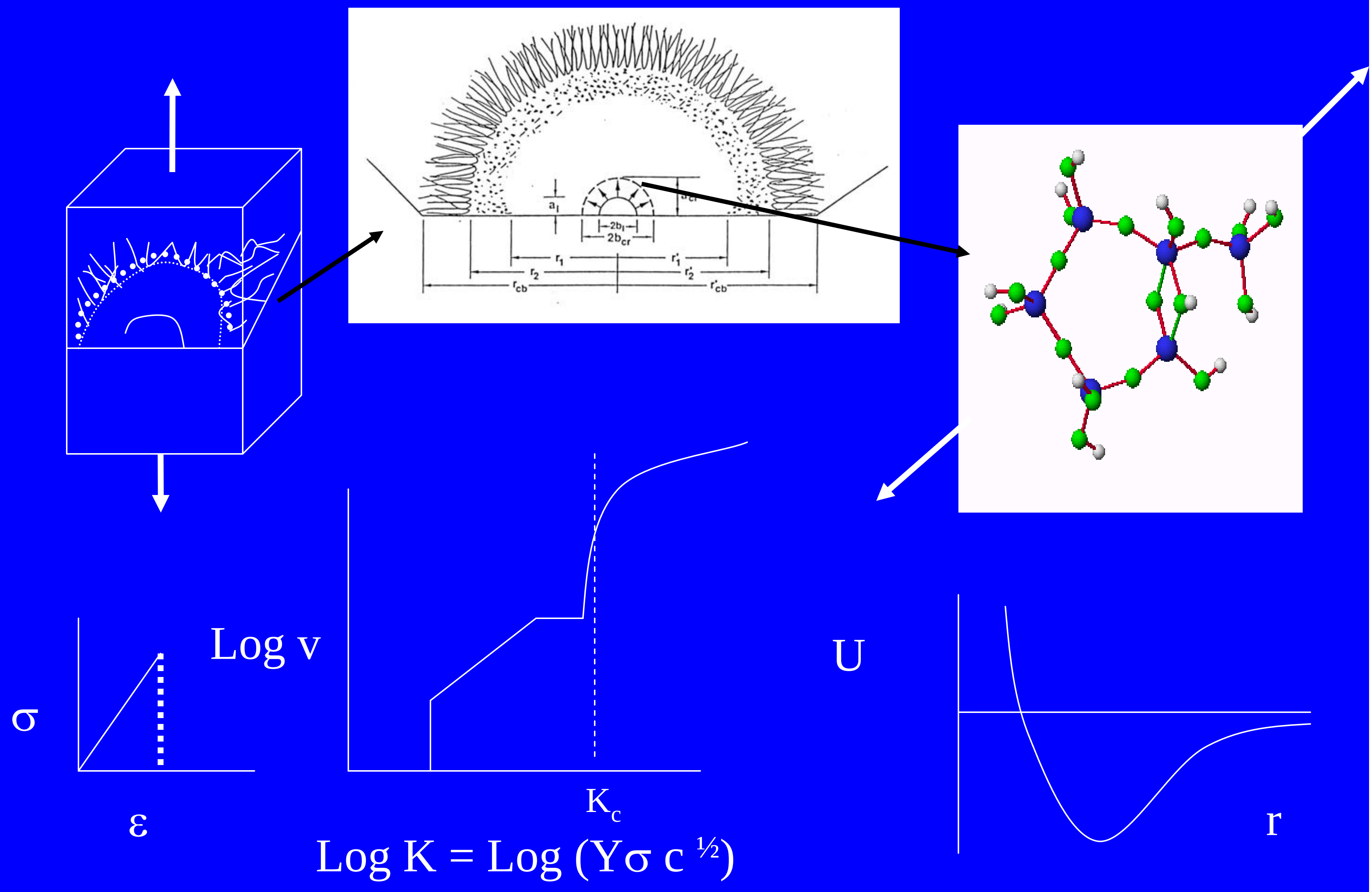
Critical Questions Need To Be Asked

- What are the energetic & geometric steps to fracture?
- Is a flat fracture (of primary bonds) possible above absolute zero? What is bond rupture?
- Is roughness a meaningful parameter in fracture?
- How does energy scale?
- How does a crack propagate at all length scales?

CONCLUSIONS

- Fractal fracture implies that the same fracture process should be able to be observed at all length scales.
- Experimental data & analytical modeling have to be interactive to be successful.
- All models should be compared to (real) experimental data.
- Analytical models have to explain fractal nature of fracture, mirror, mist & hackle and crack branching.

Bond Breaking Leads to Characteristic Features



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