

# Classical polarizable model for simulations of water and ice: Supplementary material (data)

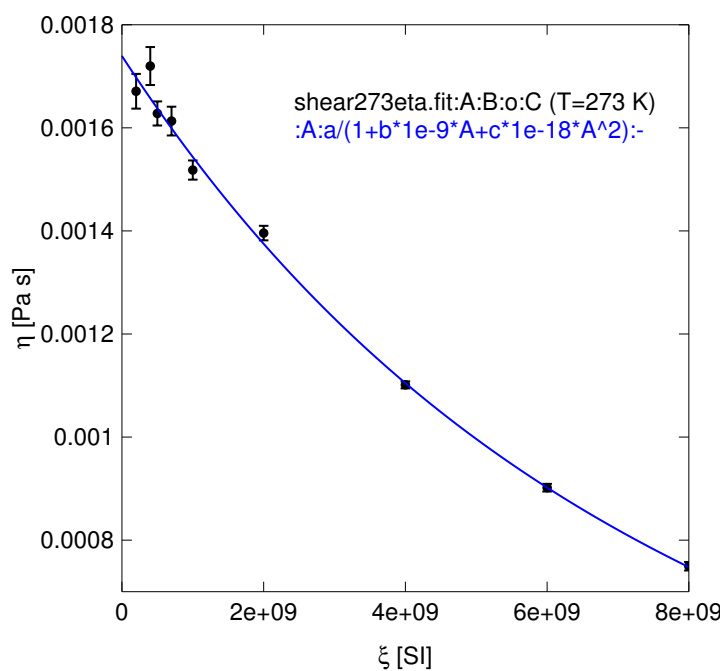
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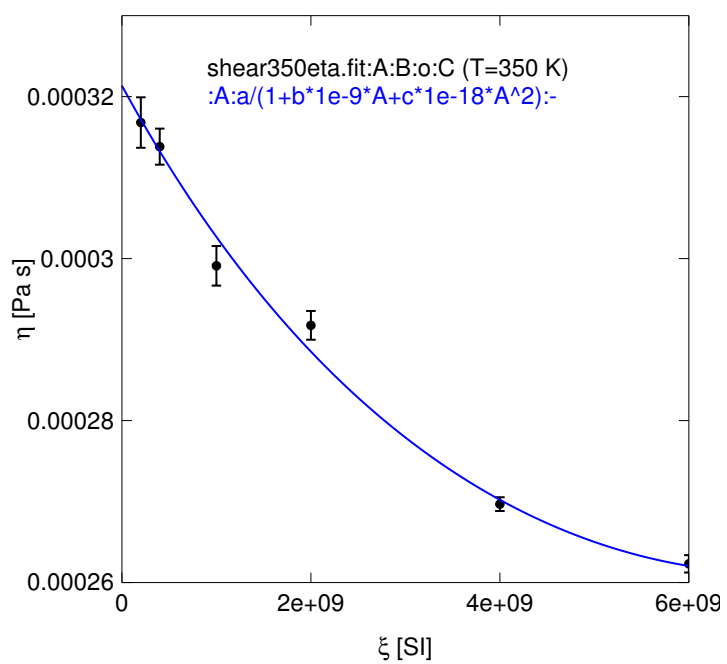
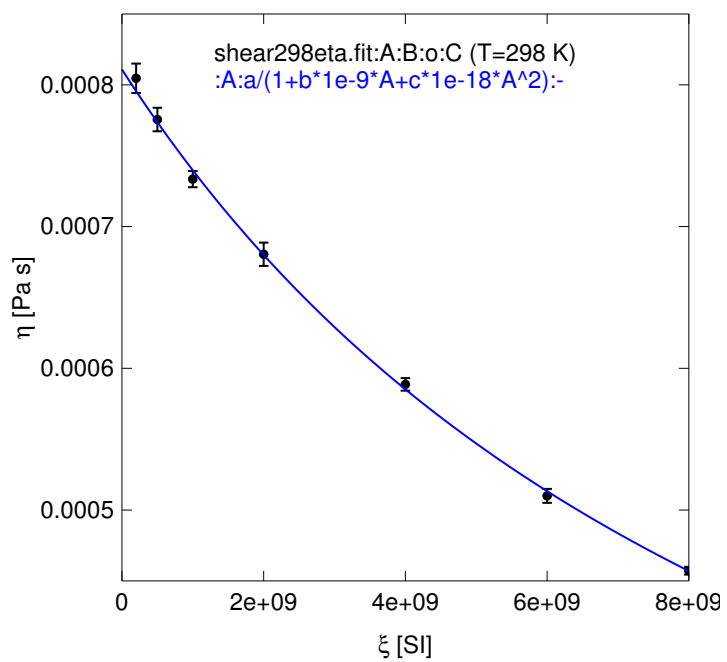
## Viscosity from NEMD

The following three pictures show the shear viscosity as a function of parameter  $\xi = \dot{T}\eta$ . The force amplitude is

$$C_f = \sqrt{\frac{8\pi^2\xi N_f k}{V L_z^2 \rho^2}}.$$

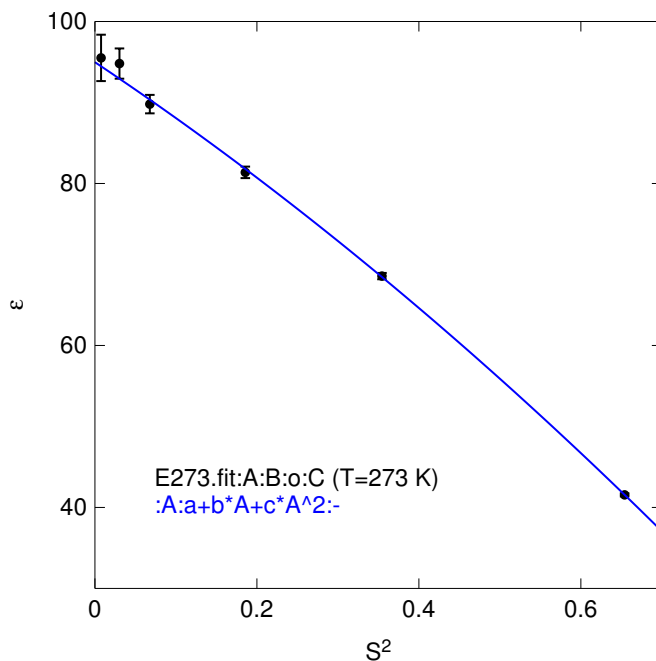
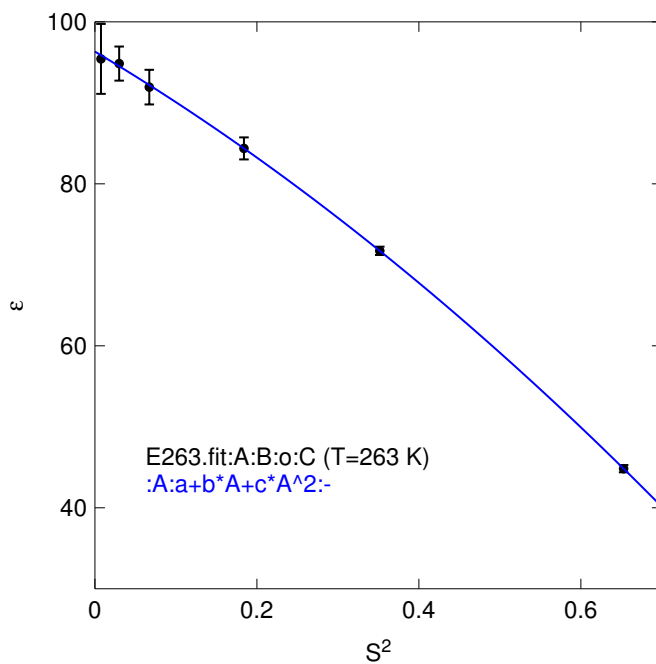
The final value is the  $\xi \rightarrow 0$  limit determined from the quadratic fit.





## Dielectric constant from external field

The following pictures show the dielectric constant as a function of squared saturation. The final value is the  $\varepsilon \rightarrow 0$  limit determined from the quadratic fit.

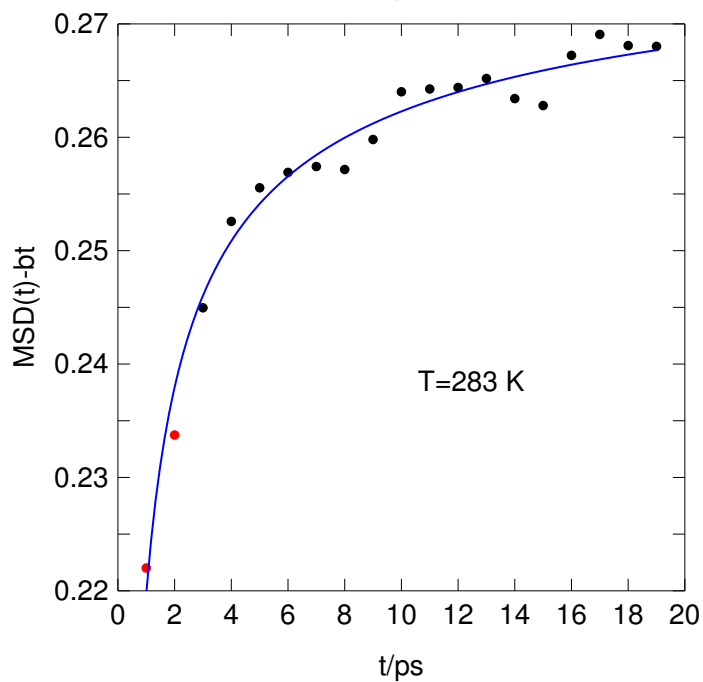
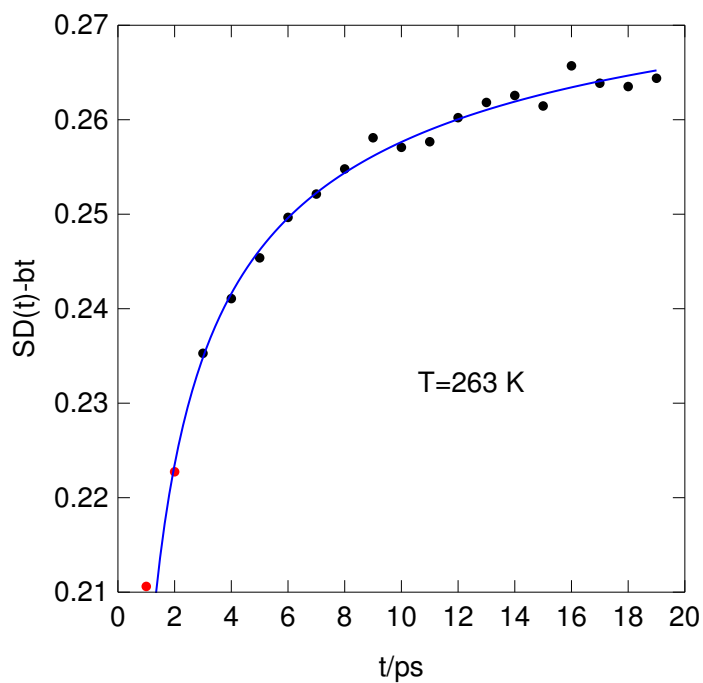


## Determinantion of diffusivity

The following pictures show functions

$$\langle SD(t) \rangle - bt$$

i.e., the squared displacement with removed linear part. The red points were not included in the fit. It is seen that  $MSD(t) = a + bt + ct^{-1/2}$  is an appropriate function to analyze the diffusion data.



## Dielectric constant summary

Numbers in parentheses are estimated standard errors in the units of the last significant digit.

$T/\text{K}$	$\epsilon_r$	$\epsilon_r^\infty$	comment
Fluctuation formula, $N = 360$ :			
263.005	97.2(27)	1.70454(14)	
273.053	91.8(24)	1.70495(12)	
282.998	88.1(21)	1.70368(10)	
298.041	82.1(15)	1.69930(6)	
319.964	76.5(14)	1.68906(7)	
349.802	64.4(8)	1.66914(4)	
273.001	103.9(30)	1.73894(9)	100 MPa
Of these, thermostats separately:			
272.996	92.2(32)	1.70503(13)	Berendsen
273.150	91.0(36)	1.70481(23)	Nosé-Hoover
297.982	81.2(19)	1.69936(6)	Berendsen
298.150	83.8(25)	1.69919(13)	Nosé-Hoover
External field, $N = 500$ :			
263	96.3(15)		
273	95.0(11)		