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Erratum: Origin of Spontaneous Electric Dipoles in Homonuclear Niobium Clusters [Phys. Rev. Lett. 93, 246105 (2004)]

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The asymmetry of the classical deflection profiles was exaggerated due to an error in the numerical simulation. Figure 1, which should replace Fig. 5 of the original Letter, shows the classical deflection of Nb_{12} approximated as a symmetric rigid body, with inertial moments $I_1 = I_2 \equiv I_{12} \neq I_3$. The method used to generate these profiles involves the discrete sampling of Eq. (23) in Ref. [1] using the parameters in Table I. For each deflection profile 10^7 random configurations $\{\theta, \dot{\theta}, \dot{\phi}, \dot{\psi}\}$

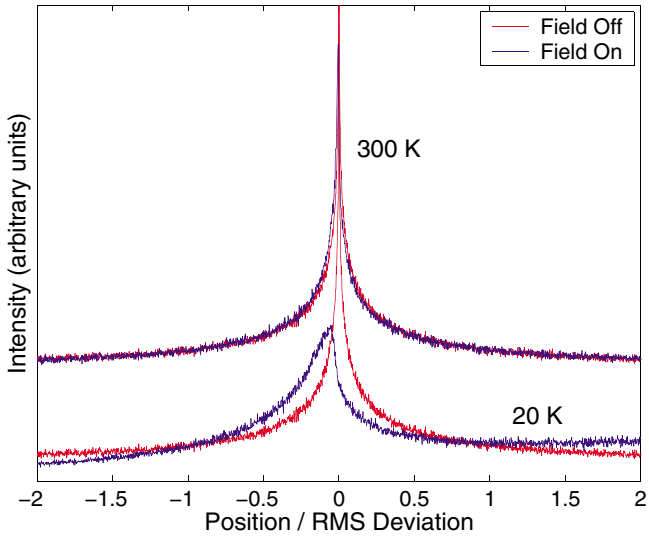

FIG. 1 (color online). Classical deflection of a model Nb_{12} cluster with a dipole moment $\mu = 2\ D$ at 300 K (top, displaced for clarity) and 20 K (bottom). At higher temperatures, the rotational dynamics masks the permanent dipole moment.

TABLE I. The parameters, in the notation of Ref. [1], K (m^2), M (M_{Nb}), I_{12} (M_{Nb} Å^2), I_3 (M_{Nb} Å^2), μ (D), F (kV/cm), and ∇F (kV/cm^2) used to generate Fig. 1 ($1M_{Nb} = 1.5427 \times 10^{-25}$ kg). The velocity $v = v(T)$ of the clusters depends on temperature T (K) as $v(20) = 300$ m/s and $v(300) = 1100$ m/s.

K	M	I_{12}	I_3	μ	F (field on)	F (field off)	∇F (field on/off)
0.165	12	45	65	2	80	0	170

were sampled with the angular velocities $\{\dot{\theta}, \dot{\phi}, \dot{\psi}\}$ bounded by $5\sqrt{2k_BT/(I_{12} + I_3)}$. The original interpretation that thermal averaging affects the symmetry of the deflection profile, leading to more asymmetry at lower temperatures, is still supported by the numerical simulations. The conclusion that thermal averaging reduces the asymmetry and thereby masks the electric dipole at higher temperatures is supported by more extensive calculations and thus remains valid.

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