Comment on the Maximum in the Loss Permittivity for the Havriliak−Negami Equation

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In a recent paper by Pathak et al.[1] experimental dielectric data are fitted to Havriliak−Negami's (HN) equation, as is quite usual nowadays. Pathak et al. actually fitted their data to a sum of two H−N functions. The authors write (p 2556): "To facilitate comparisons with literature data we determine the relaxation time τ_{max} associated with the maximum of each mode, from the H−N fitting parameters in the usual way (ref 66)". In the former sentence ref 66 refers to an earlier paper by Alvarez et al.[2] where the following formula appears

$$\tau_{max} = \tau_{HN}\left[\tan\left(\frac{\pi}{2(\beta+1)}\right)\right]^{-1/(1-\alpha)} \quad (1)$$

where α and β are the parameters appearing in the H−N equation, which reads

$$\epsilon^* = \epsilon_\infty + \frac{\Delta\epsilon}{(1+(i\omega\tau_{HN})^{1-\alpha})^\beta} \quad (2)$$

However, eq 1 is incorrect as can be seen after calculation of the maximum of the imaginary part of eq 2. The correct equation has been recently published by van Turnhout et al.[2] and Donth et al.[3] and reads

$$\tau_{max} = \tau_{HN}\left[\frac{\sin\left(\frac{\pi(1-\alpha)\beta}{2(\beta+1)}\right)}{\sin\left(\frac{\pi(1-\alpha)}{2(\beta+1)}\right)}\right]^{1/(1-\alpha)} \quad (3)$$

In a recent book Havriliak and Havriliak[5] do not give a conclusive expression for the maximum in the loss permittivity.

Incidentally, if in eq 3 one sets $\alpha = 0$, the following equation is obtained

$$\tau_{max} = \tau_{DC}\left[\tan\left(\frac{\pi}{2(\beta+1)}\right)\right]^{-1} \quad (4)$$

which is in fact the corresponding value for the maximum in the loss permittivity for a Davidson−Cole equation to which the subindex DC refers.

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References and Notes

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