From: "Leamy, Michael J" <michael.leamy@me.gatech.edu>
Subject: **RE: Correction - (10,0) zigzag torus, 12,000 atoms**
Date: July 6, 2012 3:50:31 PM EDT
To: "'Mark Jack'" <mark.a.jack@gmail.com>
Cc: "'Mario Encinosa'" <mencinosa1@comcast.net>
2 Attachments, 673 KB

This torus is better behaved since it isn't such a tight curve. Here are the results.

Best, Mike

Frequency of chosen mode (Hz) =

f =

5.716007297764718e+010

ans =

Occupation number at 300 K =

n_occup =

108

ans =

Maximum amplitude (Angstrom) of the phonon at 300 K is:

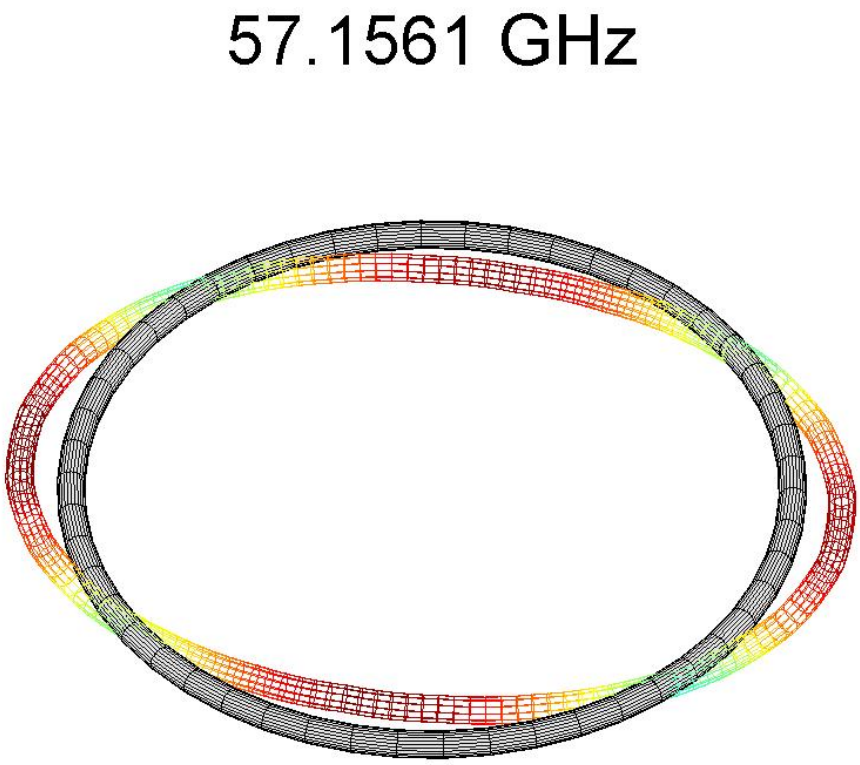
a =

0.290852452390767

-----Original Message-----
From: Mark Jack [mailto:mark.a.jack@gmail.com]
Sent: Friday, July 06, 2012 2:59 PM
To: Michael J Leamy
Cc: Mario Encinosa
Subject: Correction - (10,0) zigzag torus, 12,000 atoms

> (10,0) zigzag torus, 12,000 atoms
>
> 20 atoms for minor circumference, 600 atoms for each large ring along major circumference
>
> Torus radius (central radius, R): 101.47 Angstrom
>
> Tube radius (torus width, a): 3.90566 Angstrom
>
> Electronic hopping parameter: -3.1 eV
>
> Electron-phonon coupling: +5.3 eV / Angstrom
>
> See phi-theta coordinates attached.
>
> M.

c 12000 atoms, 20 atoms per small rings (width), 600 atoms per large ring:
c bigr = 1.4168*600/4*3/2/pi = 101.47
c smallr = 1.4168*20/2*sqrt(3)/2/pi = 3.90566
bigr = 101.47d0
smallr = 3.90566d0



PhononDispl....txt (599 KB)