**From:** "Leamy, Michael J" <michael.leamy@me.gatech.edu>
**Subject:** **RE: Correction - (10,10) armchair torus, 12,000 atoms**
**Date:** July 6, 2012 3:38:21 PM EDT
**To:** "'Mark Jack'" <mark.a.jack@gmail.com>
**Cc:** "'Mario Encinosa'" <mencinosa1@comcast.net>
2 Attachments, 708 KB

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Ok, here are some results for the first bending mode of the 10,10 at 34.7GHz. This torus radius is pretty tight and gave my code some troubles. Basically, the lattice will need to be relaxed in order to make a torus this tight, and I haven't done that step. It would take me some effort to implement such a procedure. For now, I did get the first bending mode ok, but the higher modes had imaginary frequencies due to negative stiffnesses associated with the tight torus radius.

The file attached has the displaced (X,Y,Z) coordinates of the atoms.

Frequency of chosen mode (Hz) =

f =

3.473052528476825e+010

ans =

Occupation number at 300 K =

n_occup =

179

ans =

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

a =

0.536169730522313

-----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 - (10,10) armchair torus, 12,000 atoms

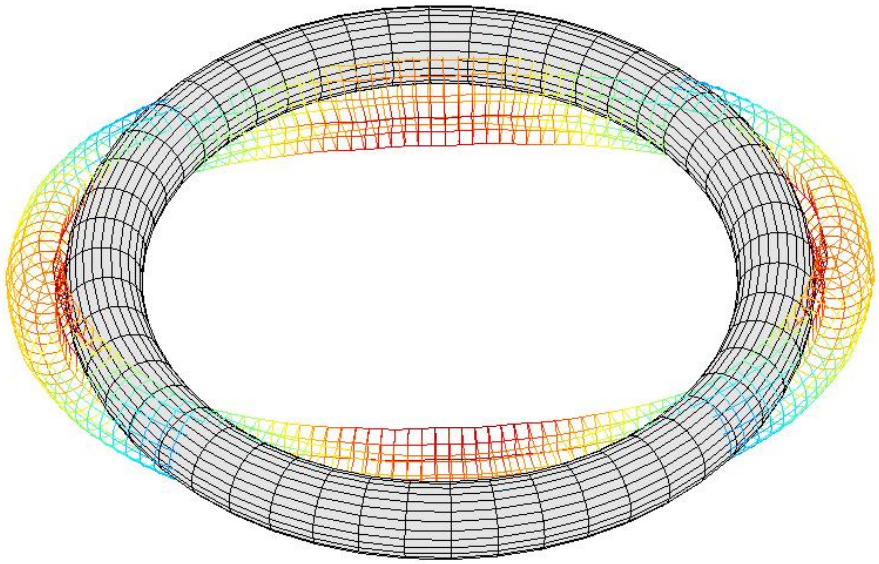
> (10,10) armchair torus, 12,000 atoms
>
> 40 atoms for minor circumference, 300 rings around major circumference
>
> Torus radius (central radius, R): 58.58 Angstrom
>
> Tube radius (a): 6.76481 Angstrom
>
> Electronic hopping parameter: -3.1 eV
>
> Electron-phonon coupling: +5.3 eV / Angstrom

> See theta-phi coordinates attached.
>
> M.

c 12000 atoms, 300 rings, 40 atoms per small ring, (10,10) armchair torus:

```
c     bigr   = 1.4168*300/2*sqrt(3)/2/pi = 58.58
c     smallr = 1.4168*40/4*3/2/pi = 6.76481
      bigr = 58.58d0
      smallr = 6.76481d0
```

34.7281 GHz



PhononDispl....txt (599 KB)