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## Local vibrations of thermal double donors in silicon

Y. J. Lee, M. Pesola, J. von Boehm, and R. M. Nieminen

*COMP/Laboratory of Physics, Helsinki University of Technology, P.O. Box 1100, FIN-02015 HUT, Finland*

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The local vibrational modes (LVM's) of the oxygen chains assigned to thermal double donors (TDD's) and other related oxygen defects in silicon are studied using accurate total-energy calculations. We find that the calculated LVM frequencies as well as their isotopic shifts and charge-state dependences (temperature dependences) for the oxygen chains agree closely with the corresponding experimental quantities, which supports our assignments of the  $O_{2i}-O_{2r}$  chain to TDD1 and the  $O_i-O_{nr}-O_i$  chains to TDD $n$  ( $n > 1$ ) ( $O_i$  is an interstitial oxygen and  $O_r$  a threefold coordinated oxygen belonging to a ring).

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Since their first discovery in 1954 (Ref. 1) thermal double donors (TDD's) in silicon have attracted constant interest due to their peculiar properties and technological importance. TDD's form a family of at least 17 closely related members (TDD0–TDD16) (Refs. 2–4) and appear consecutively under thermal heating at 350–550°C.<sup>2,5</sup> The structures of TDD's have long remained unclear but are commonly believed to consist of aggregated oxygen due to oxygen supersaturation in Czochralski-grown silicon. An important achievement in finding these structures as well as in clarifying the consecutive mechanism between the TDD's was the assignment of the infrared absorption local vibrational modes (LVM's) of 975, 988, 999, and 1006  $\text{cm}^{-1}$  to TDD1, TDD2, TDD3, and TDD4, respectively.<sup>6–8</sup> Also the isotopic shifts when  $^{16}\text{O}$  is replaced by  $^{18}\text{O}$  have been measured: the shifts are  $-43$ – $-44$   $\text{cm}^{-1}$ .<sup>8</sup> The LVM frequencies on one hand act as useful fingerprints in following the kinetics of TDD's, and on the other hand serve as a stringent test for structural models for TDD's.

It has been suggested both experimentally<sup>9</sup> and theoretically<sup>10</sup> that an interstitial Si atom should be involved in the cores of the TDD's. However, more recent total-energy calculations indicate that oxygen-only structures for TDD's are those energetically most favorable.<sup>8,11–13</sup> On the basis of accurate total-energy calculations we recently put forward an oxygen-chain-like model for TDD's.<sup>13</sup> This consists of adjacent four-member rings ( $R$ 's) and flanking interstitial oxygens ( $O_i$ 's). The  $R$  unit consists of two threefold coordinated O atoms ( $O_r$ 's) bonded to two common Si atoms.<sup>14</sup> The O chains obtained by us for TDD0, TDD1, and TDD $n$  ( $n > 1$ ) are  $O_i-O_{2r}$ ,  $O_{2i}-O_{2r}$ , and  $O_i-O_{nr}-O_i$  ( $n > 1$ ), respectively.<sup>13</sup>

We have shown that a rate-equation model for the O chains is able to produce the experimentally observed annealing kinetics of the TDD's.<sup>15,16</sup> However, the agreement may depend on the parameters we use in the kinetic model. It is therefore of paramount importance to compare the calculated LVM frequencies and modes of the O chains directly with the corresponding experimental quantities for the TDD's.

The aim of this paper is to report calculated LVM's for the O chains. We find that the relevant calculated LVM frequencies originate from the asymmetric stretching vibrations of the flanking  $O_i$ 's of the O chains and agree systematically with the experimental LVM frequencies quoted above.

The total-energy calculations are performed using the self-consistent plane-wave pseudopotential method (PP).<sup>17</sup> For Si we use the norm-conserving Hamann PP.<sup>18</sup> The PP is of the fully separable Kleinman-Bylander form<sup>19</sup> and the  $s$  component is used as the local one. For O we use the ultrasoft Vanderbilt PP.<sup>20</sup> A kinetic-energy cutoff of 28 Ry and the  $\Gamma$ -point sampling are used. We use an elongated 162-atom-site supercell that gives an intercell distance of 35 Å along the [110] direction of the O chains. All ionic coordinates are allowed to relax without any constraints until the largest remaining Hellmann-Feynman force component is less than 0.1 meV/Å. However, in the case of the  $O_{2i}-O_{2r}$  chain we had difficulties in stabilizing the ground-state structure for reasons that are not clear to us. Therefore, in this case we use an elongated 108-atom-site supercell that gives an intercell distance of 22 Å along the [110] direction. The procedure and program by Köhler *et al.*<sup>21</sup> used earlier for  $O_i$  and vacancy-oxygen complexes,<sup>22–24</sup> are used in calculating the present LVM's. Every atom vibrating in an LVM is displaced to all six Cartesian directions from its equilibrium position, the electronic structure for this configuration is optimized, and the resulting Hellman-Feynman forces are calculated. The coupling constants for the dynamical matrix are formed from these forces and displacements. Since we are interested in localized modes it is sufficient to include in the calculations only those atoms that have a significant vibrational amplitude. We have tested this approximation systematically for  $O_{3i}$ ,  $O_i-O_{2r}$ , and  $O_{2i}-O_{2r}$ . It turns out that the inclusion of only the flanking Si- $O_i$ -Si-O atom group results in an error less than 2  $\text{cm}^{-1}$ . At least these four atoms are always included in the LVM calculations.

The calculated highest LVM frequencies for the O chains are given in Table I together with the experimental frequencies and the frequencies calculated by Coutinho *et al.*<sup>8</sup> The calculated LVM frequencies related to TDD's are given for the doubly positive charge state of the corresponding O chain because almost all TDD's have donated two electrons to the conduction band at temperatures  $T > 100$  K (for the  $O_i-O_{2r}$  chain  $T > 200$  K). We first note that by increasing the size of the supercell from 32 to the present 162 atom sites we find a closer agreement with the experimental LVM frequencies for monomers and dimers: for  $O_i$   $1098 \rightarrow 1138$   $\text{cm}^{-1}$  (experiment 1136  $\text{cm}^{-1}$ ) and for  $O_{2i}$   $1033, 984 \rightarrow 1043$ ,

TABLE I. High-lying LVM frequencies ( $\text{cm}^{-1}$ ) for thermal double donors and related oxygen chains in silicon. The isotopic shifts, when  $^{16}\text{O}$  is replaced by  $^{18}\text{O}$ , are given in parenthesis. The value for the  $\text{O}_i\text{-O}_{5r}\text{-O}_i^{2+}$  chain is an estimate.

Structure	This work	Experiment	Coutinho <i>et al.</i> <sup>a</sup>
$\text{O}_i^0$	1138	1136 <sup>b</sup>	
$\text{O}_{2i}^0$	1043(-48)	1060(-48) <sup>c</sup>	
	1013(-44)	1012(-43) <sup>d</sup>	
$\text{O}_{3i}^0$	1072(-49)		
	987(-45)	1005 <sup>e</sup>	
	945(-41)		
$\text{O}_i\text{-O}_{2r}^{2+}$	973(-43)		
$\text{O}_{4i}^0$	1010(-46)	1020 <sup>f</sup>	
	955(-44)		
	920(-41)		
$\text{O}_{2i}\text{-O}_{2r}^{2+}$	978	975 <sup>g</sup> (TDD1)	940 ( $\text{O}_5$ )
	942		
$\text{O}_i\text{-O}_{2r}\text{-O}_i^{2+}$	992(-45)	988(-43) <sup>g</sup> (TDD2)	951 ( $\text{O}_6$ )
$\text{O}_i\text{-O}_{3r}\text{-O}_i^{2+}$	988(-45)	999(-44) <sup>g</sup> (TDD3)	963 ( $\text{O}_7$ )
$\text{O}_i\text{-O}_{4r}\text{-O}_i^{2+}$	1000(-45)	1006 <sup>a</sup> (TDD4)	969 ( $\text{O}_8$ )
$\text{O}_i\text{-O}_{5r}\text{-O}_i^{2+}$	$\approx 1006$		

<sup>a</sup>Reference 8.

<sup>b</sup>References 25 and 26.

<sup>c</sup>References 27 and 28.

<sup>d</sup>References 8, 27, and 28.

<sup>e</sup>Reference 29.

<sup>f</sup>Reference 30.

<sup>g</sup>References 7 and 8.

$1013 \text{ cm}^{-1}$  (experiment  $1060, 1012 \text{ cm}^{-1}$ ).<sup>22-24</sup> Also, the calculated isotopic shifts for  $\text{O}_{2i}^0$  when  $^{16}\text{O}$  is replaced by  $^{18}\text{O}$  agree within  $1 \text{ cm}^{-1}$  with the experimental shifts (Table I).

According to the kinetic simulations<sup>15,16</sup> one of the two experimental  $1005 \text{ cm}^{-1}$  bands<sup>29</sup> should originate from an LVM of the staggered  $\text{O}_{3i}^0$  chain. The three calculated high-frequency LVM's for the staggered  $\text{O}_{3i}^0$  chain are shown in Fig. 1 (we call the modes having a frequency higher than  $900 \text{ cm}^{-1}$  high-frequency modes in the following). The highest frequency of  $1072 \text{ cm}^{-1}$  originates from the asymmetric stretching vibration of the flanking  $\text{O}_i$  bowed towards the center of the chain [Fig. 1(a)]. The next highest frequencies of  $987$  and  $945 \text{ cm}^{-1}$  originate from the coupled asymmetric stretching vibrations of the center  $\text{O}_i$  and the right flanking  $\text{O}_i$  bowed outwards from the center [Figs. 1(b) and 1(c), respectively]. The two modes in Figs. 1(b) and 1(c) resemble those of the staggered dimer.<sup>22,23</sup> The calculated frequency of  $987 \text{ cm}^{-1}$  lies closest to the experimental frequency of  $1005 \text{ cm}^{-1}$  and is thus identified with this (Table I).

Our calculations predict a LVM frequency of  $973 \text{ cm}^{-1}$  (Table I) for the highest mode of the  $\text{O}_i\text{-O}_{2r}^{2+}$  chain, assigned to TDD0.<sup>13</sup> In this mode the flanking  $\text{O}_i$  performs asymmetric stretching vibration similar to the mode shown in Fig. 1(a). To the best of the authors' knowledge no experimental frequency is available for TDD0. This

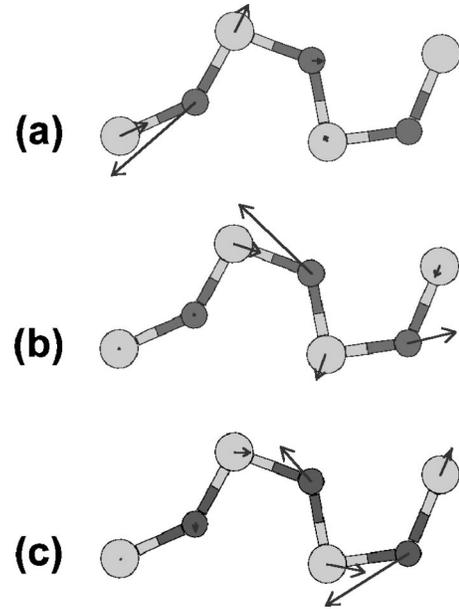


FIG. 1. The calculated highest local vibrational modes for the staggered  $\text{O}_{3i}^0$  chain: (a)  $1072 \text{ cm}^{-1}$ , (b)  $987 \text{ cm}^{-1}$ , and (c)  $945 \text{ cm}^{-1}$ . Oxygen atoms are drawn in darker gray, silicon atoms in lighter gray.

may be due to the fact that the  $\text{O}_i\text{-O}_{2r}^{2+}$  chain has about  $0.4 \text{ eV}$  higher formation energy than the staggered  $\text{O}_{3i}^0$  chain for values of the electron chemical potential above  $0.48 \text{ eV}$ .<sup>13,31</sup>

Hallberg and Lindström find experimentally that TDD1 and TDD2 form bistable systems with a common electrically inactive  $X$ -state configuration that has an IR absorption band at  $1020 \text{ cm}^{-1}$ .<sup>30</sup> On the basis of the total-energy calculations we assign the electrically inactive staggered  $\text{O}_{4i}^0$  chain to the  $X$ -state configuration.<sup>13</sup> We find that the calculated highest LVM frequency originates from the asymmetric stretching vibration of the flanking  $\text{O}_i$  similarly to the  $1072 \text{ cm}^{-1}$  mode of the staggered  $\text{O}_{3i}^0$  chain in Fig. 1(a). This highest LVM frequency is  $1010 \text{ cm}^{-1}$  and agrees closely with the experimental value of  $1020 \text{ cm}^{-1}$  (Table I).<sup>30</sup> The agreement is thus consistent with our assignment of the staggered  $\text{O}_{4i}^0$  chain to the  $X$ -state configuration.<sup>13</sup> Similarly to the staggered  $\text{O}_{3i}^0$  chain the staggered  $\text{O}_{4i}^0$  chain has also two other high-frequency modes (Table I).

The calculated two highest LVM's for the  $\text{O}_{2i}\text{-O}_{2r}^{2+}$  chain (TDD1) are shown in Fig. 2. They are qualitatively similar to the two highest LVM's of the staggered  $\text{O}_{3i}^0$  chain in Fig. 1. The higher frequency of  $978 \text{ cm}^{-1}$  originates from the asymmetric stretching vibration of the flanking  $\text{O}_i$  and agrees closely with the experimental value of  $975 \text{ cm}^{-1}$  for TDD1 (Table I).<sup>7,8</sup> This agreement is thus consistent with our assignment of the  $\text{O}_{2i}\text{-O}_{2r}$  chain to TDD1.<sup>13</sup>

The highest LVM's of the  $\text{O}_{2i}\text{-O}_{2r}^{2+}$  chain resemble those of the staggered O chains as follows. The  $\text{O}_{2i}\text{-O}_{2r}^{2+}$  chain has two adjacent flanking  $\text{O}_i$ 's that can generate two high-frequency modes (compare Figs. 1 and 2). However, a third high-frequency mode is not allowed because the third O atom ( $\text{O}_r$ ) is threefold coordinated which softens

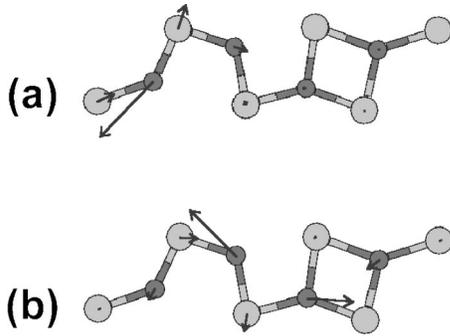


FIG. 2. The calculated highest local vibrational modes for the  $O_{2i}-O_{2r}^{2+}$  chain (TDD1): (a)  $978\text{ cm}^{-1}$  and (b)  $942\text{ cm}^{-1}$ . Oxygen atoms are drawn in darker gray, silicon atoms in lighter gray.

the third highest mode of the  $O_{2i}-O_{2r}^{2+}$  chain down to  $866\text{ cm}^{-1}$ .

The calculated highest LVM for the  $O_i-O_{2r}-O_i^{2+}$  chain (TDD2) is shown in Fig. 3(a). The LVM originates again from the asymmetric stretching vibration of the flanking  $O_i$ . The corresponding LVM frequency is  $992\text{ cm}^{-1}$  and agrees closely with the experimental value of  $988\text{ cm}^{-1}$  for TDD2 (Table I).<sup>7,8</sup> This agreement is thus consistent with our assignment of the  $O_i-O_{2r}-O_i$  chain to TDD2.<sup>13</sup> The structure in Fig. 3(a) is symmetric and the asymmetric stretching vibrations of both flanking  $O_i$ 's give the same frequency. Since the two flanking  $O_i$ 's are coupled to the threefold coordinated  $O_r$ 's other high-frequency modes do not occur and the next highest LVM frequency is softened down to  $788\text{ cm}^{-1}$  as in the  $O_{2i}-O_{2r}^{2+}$  chain.

In the same way, also the next  $O_i-O_{nr}-O_i^{2+}$  chains (TDDn,  $n>2$ ) have two similar symmetric flanking  $O_i$ 's whose asymmetric stretching vibrations give rise to one high-frequency LVM. This is shown in Fig. 3(b) for the  $O_i-O_{3r}-O_i^{2+}$  chain (TDD3). The highest calculated LVM frequencies for the  $O_i-O_{3r}-O_i^{2+}$  and  $O_i-O_{4r}-O_i^{2+}$  chains are  $988$  and  $1000\text{ cm}^{-1}$ , respectively (Table I). The calculated LVM frequencies agree closely with the corresponding experimental values of  $999$  and  $1006\text{ cm}^{-1}$  (Table I).<sup>7,8</sup> This agreement is consistent with our assignment of the

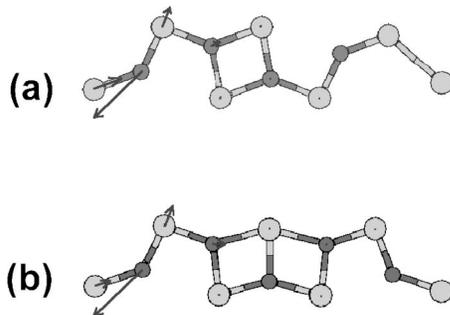


FIG. 3. The calculated highest local vibrational modes for the  $O_i-O_{2r}-O_i^{2+}$  chain (TDD2,  $992\text{ cm}^{-1}$ ) (a) and the  $O_i-O_{3r}-O_i^{2+}$  chain (TDD3,  $988\text{ cm}^{-1}$ ) (b). Oxygen atoms are drawn in darker gray, silicon atoms in lighter gray.

TABLE II. Calculated LVM frequency shifts ( $\text{cm}^{-1}$ ) when the charge state changes from doubly positive to neutral for  $O_i-O_{2r}$  ( $n=0$ ), and  $O_i-O_{nr}-O_i$  ( $n>1$ ). The shifts for the  $^{18}\text{O}$  isotope chains are given in parentheses.

$n$	0	2	3	4
Shift	5(4)	17(16)	10(9)	12(11)

$O_i-O_{nr}-O_i$  chains to TDDn ( $n>2$ ).<sup>13</sup> However, the calculated frequency for the  $O_i-O_{3r}-O_i^{2+}$  chain ( $988\text{ cm}^{-1}$ ) is lower than that for the  $O_i-O_{2r}-O_i^{2+}$  chain ( $992\text{ cm}^{-1}$ ) whereas the corresponding experimental frequency for TDD3 ( $999\text{ cm}^{-1}$ ) is by  $11\text{ cm}^{-1}$  higher than that for TDD2 ( $988\text{ cm}^{-1}$ ). We believe that this inconsistency is due to the insufficient  $\mathbf{k}$ -point sampling (we use only  $\Gamma$  point).

Coutinho *et al.* have reported LVM frequencies for O chains, summarized in Table I.<sup>8</sup> Even though the calculated differences between the adjacent LVM frequencies agree closely with the corresponding experimental differences between TDD's in Table I, the calculated frequencies lie about  $35\text{ cm}^{-1}$  below the experimental ones, showing a less satisfactory agreement. Coutinho *et al.* assign  $O_{4+n}$  to TDDn, which differs from our assignments given in Table I in that we have less O atoms in our corresponding chains: 4 O atoms in TDD1 and TDD2,  $2+n$  O atoms in TDDn for  $n>2$ . The experimental kinetic study by Åberg *et al.* indicates that TDD2 forms directly from TDD1 via reconfiguration.<sup>29</sup> Both TDD1 and TDD2 are found experimentally to be bistable with the *same* electrically inactive X state,<sup>30</sup> showing that these structures are closely related and are probably different configurations of the same complex. These experimental findings are difficult to explain if TDD1 and TDD2 have a different number of O atoms as is the case in the model by Coutinho *et al.*, but are natural to understand with our O chain model where  $O_{2i}-O_{2r}$  (TDD1),  $O_i-O_{2r}-O_i$  (TDD2), and (the staggered)  $O_{4i}$  (the X state) are different configurations of the same  $O_4$  complex.<sup>13,15,16</sup>

At low temperatures the electrons donated to the conduction band return to the TDD's making them electrically neutral (the TDD's change from the doubly positive state to the 0 state). It may be expected that the LVM frequencies of the TDD's undergo a positive shift when  $T$  becomes low because two more localized electrons strengthen the interatomic bonding. In fact, it is found experimentally that the  $975$  (TDD1),  $988$  (TDD2),  $999$  (TDD3), and  $1006\text{ cm}^{-1}$  (TDD4) frequencies *increase* by about 3, 3, 3, and  $0.5\text{--}1\text{ cm}^{-1}$ , respectively, when  $T$  decreases from the room temperature to 10 K (Ref. 32) whereas during the same temperature change the experimental  $1060$  and  $1012\text{ cm}^{-1}$  frequencies ( $O_{2i}$ ) decrease slightly (2 and  $0\text{--}0.6\text{ cm}^{-1}$ , respectively).<sup>32,33</sup> This behavior may be understood qualitatively by means of the change in the charge state. The calculated frequencies for the  $O_i-O_{2r}$  (TDD0) and  $O_i-O_{nr}-O_i$  (TDDn,  $n>1$ ) chains all undergo—similar to the experiments—positive shifts when the charge state changes from doubly positive to neutral (Table II). On the other hand,  $O_{2i}$  does not have a donor state and  $O_{2i}$  remains, therefore, always neutral. As a consequence the calculated frequencies for  $O_{2i}$  (Table I) also remain con-

stant in qualitative agreement with the experiments<sup>32,33</sup>. (We do not expect here a quantitative agreement because all calculations are performed at 0 K.)

In conclusion, we find that the calculated LVM frequencies as well as their isotopic shifts and charge-state dependences (temperature dependences) for the oxygen chains agree closely with experiments and support our assignments of the  $O_{2i}-O_{2r}$  chain to TDD1 and the  $O_i-O_{nr}-O_i$  chain to

TDDn ( $n > 1$ ) as well as the staggered  $O_{4i}$  chain to the X state.

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