Theoretical Properties of Ni$_2$Ti alloys Studied: by Gaussian 09 Program

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Abstract. The results obtained from theoretical calculations using the Gaussian 09 program using density functional (DFT) theory through calculated each of structural, electronic, thermal, and mechanical properties such as Poisson's ratio, Young's modulus, and shear modulus from the elastic constants calculated for Ni$_2$Ti. Also, that prepared these alloys and tested on people of both sexes to learn how important it is to improve orthodontic treatments and found that the results obtained in experimental and theoretical compatible to some extent.

Keywords: DFT, Electronic Properties, Orthodontics.

1. Introduction

Orthodontics is the branch of dentistry that modifies teeth and jaws that are positioned improperly. The benefits of orthodontic treatment include a healthier mouth, a more pleasing appearance, and teeth that are more likely to last a lifetime$^{[1]}$. So that starting of the treatment process for overseas and prominent upper teeth in children without the wait until the child has reached adolescence has been shown to reduce damage to the lateral and central incisors$^{[2]}$.

The orthodontics is a wire conforming to the alveolar or dental arch that can be used with dental braces as a source of force in correcting irregularities in the position of the teeth. An archwire can also be used to maintain existing dental positions; in this case, it has a retentive purpose$^{[3]}$. Orthodontic archwires may be fabricated from several alloys, most commonly stainless steel, nickel-titanium alloy (Ni$_2$Ti), and beta-titanium alloy (composed primarily of titanium and molybdenum)$^{[4]}$. The composition of the wire has 55% Nickel and 45% Titanium$^{[4]}$. The main goal of this research is to study the theoretical properties of Ni$_2$Ti after that used these materials on the orthotics since.

2. Methods and Materials

The experimental part included theoretical calculations using Gaussian09 program, B3LYP functional is frequently described as one of the successful methods within the framework of density functional theory (DFT) which was used in the present work in combination with the appropriate basis to get each of structural, spectrum properties (FTIR) and each of mechanical and thermal characteristics depending on the equation, so that ionization potential (IP) and electron affinity (EA) have been calculated by using equations.
IP= - EHOMO ... (1)
EA= - ELUMO ... (2)
While the electronegativity ($\chi$) has been calculated by using the following equation
$$\chi = - (IP + EA)/2 \ldots (3)$$
Whereas the hardness ($\eta$) is defined as
$$\eta = (IP - EA)/2 \ldots (4)$$
The softness (S) and electrophilic (W) by the following equations 5 and 6.
$$S= 1/2\eta \ldots (5)$$
$$W= \chi^2/2\eta \ldots (6)$$

In addition, in the experimental part, which includes preparing extracts of Ni$_2$Ti by taking (20 ml) of dried and ground Miswak, and adding (120 ml) of ethyl alcohol its purity is (99.98%). The mixture soaks for 16 hours and filtered to obtain the extract. This process must be repeated four times to ensure the process. The leachate is then placed in the rotary evaporator and the extraction process is carried out at 45 °C.

This research was done in the medical city of Baghdad by examining the six samples of orthodontics and for each three were applied by Ni$_2$Ti extract. Each of the six samples was examined by a microscope in the laboratories to know their effects on bacteria on them.

3. Results and Discussions:
Figure (1) showed the optimization structure, i.e., the formed molecular

![Figure 1. Optimization structure of Ni$_2$Ti](image)

The electronic structures of alloy include calculation of energy gaps where the figure (2) showed each of Homo and Lumo states

![Figure 2. The energy gap.](image)

While FTIR gives information about the chemical bonding between Ni$_2$Ti so that, a series of absorption peaks from (0 to 500) cm$^{-1}$ can be found, as illustrated in figure (3).
Table 1. Showed electronics, mechanical and thermal properties

| Mechanical properties | Thermal properties |
|-----------------------|--------------------|
| IP                    | 6.4835             |
| EA                    | 6.09499            |
| K                     | 6.2893             |
| D                     | 0.194286           |
| S                     | 0.0097143          |
| W                     | 101.7956           |
| Temperature           | 298.1 K            |
| Pressure              | 1.0000 atm.        |
| Frequencies           | 0.8929             |
| Electronic Energy     | -3191.49 Hartree   |

Thermal properties
- Thermal Correction to Energy: 0.006647 Hartree
- Thermal Correction to Enthalpy: 0.007591 Hartree
- EE+ Zero-Point energy: -0.023898 Hartree
- EE+ Enthalpy Correction: -3191.5148 Hartree
- EE+ Free Energy Correction: -3191.518 Hartree
- Thermal Capacity (Cv): 11.936 cal/mol
- Entropy (S): 66.274 cal/mol
- Temperature: 4.171 kcal/mol

Table 2. Showed percentage of reduction of the two groups of samples.

| Reduction percentage | Treated by                | Sample                      |
|----------------------|---------------------------|-----------------------------|
| 60-75                | Ni2Ti extract             | First group (1,2,3 samples) |
| 50-60                | Ni2Ti extract +Toothpaste | Second group (4,5,6 samples)|

Table 3. Comparison between female and male for twice used Ni2Ti

| Reduction percentage | Out of 100% | Treated by                | Gender(M: male , F: female) | Total | Times of brushing (times per day) |
|----------------------|-------------|---------------------------|----------------------------|-------|-----------------------------------|
| 0%                   | 100%        | Ni2Ti extract             | M                          | 2     | ½/ day                            |
| 30%                  | 70%         | Ni2Ti extract +Toothpaste | F                          | 1     | 1/ day                            |
| 45%                  | 55%         | Ni2Ti extract             | F                          | 2     | 2/ day                            |
| 60%                  | 40%         | Ni2Ti extract +Toothpaste | M                          | 1     | 3/day                             |

Results: Results indicate that there is no significant difference in bacterial growth on the Orthodontics neither for both males and females nor for different ages. As shown in table (2), (3) of bacterial growth on the Orthodontics neither for both male and female nor for different ages.
4. Conclusions

The theoretical properties that were calculated through the use of the Gaussian program gave an impression about that material to be used in this application because it was distinguished by all that the template needs from thermal and mechanical properties, which strengthened the application side before starting it.

5. References

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