

Adaptive Design of Metallic Nanoscale Chains

Amy Cassidy, Stephan Haas
Department of Physics and Astronomy
Ilya Grigorenko, A.F.J Levi
Department of Electrical Engineering
University of Southern California

15 January 2006

Surface Plasmons

- What are they?
 - Collective excitations of electrons in the presence of an external electric field
 - Strongly enhance local electric field at metal surface
- Why are they interesting?
 - Optical Waveguides
 - Using surface plasmons in metal nanoparticles to transport energy:
 - through sub-wavelength structures.
 - around sharp corners with little loss.
 - Single Photon Source
 - Biosensors



Plasmon wave guide from d~50 nm gold dots.

Maier, *et al.* *Adv. Mater.* **2001**, 13, No 19.

Dielectric Function, $\epsilon(\mathbf{q}, \omega)$

- Describes the response of the system to external fields.
- In the Random Phase Approximation,

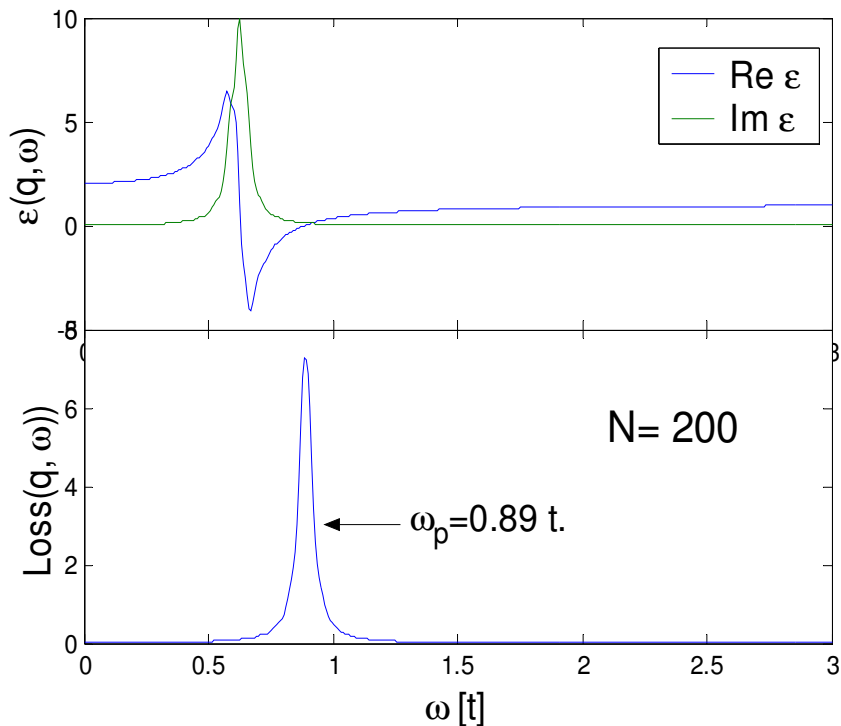
$$\epsilon(\mathbf{q}, \omega) = 1 - V(\mathbf{q}) \frac{1}{V} \sum_{i,j} \frac{f(E_i) - f(E_j)}{\omega - E_i + E_j} |\langle i | e^{i\mathbf{q} \cdot \mathbf{r}} | j \rangle|^2$$

– With $V(\mathbf{q}) = \frac{e^2}{2\pi\epsilon_0} \ln \frac{1}{qa}$ for a 1D system.

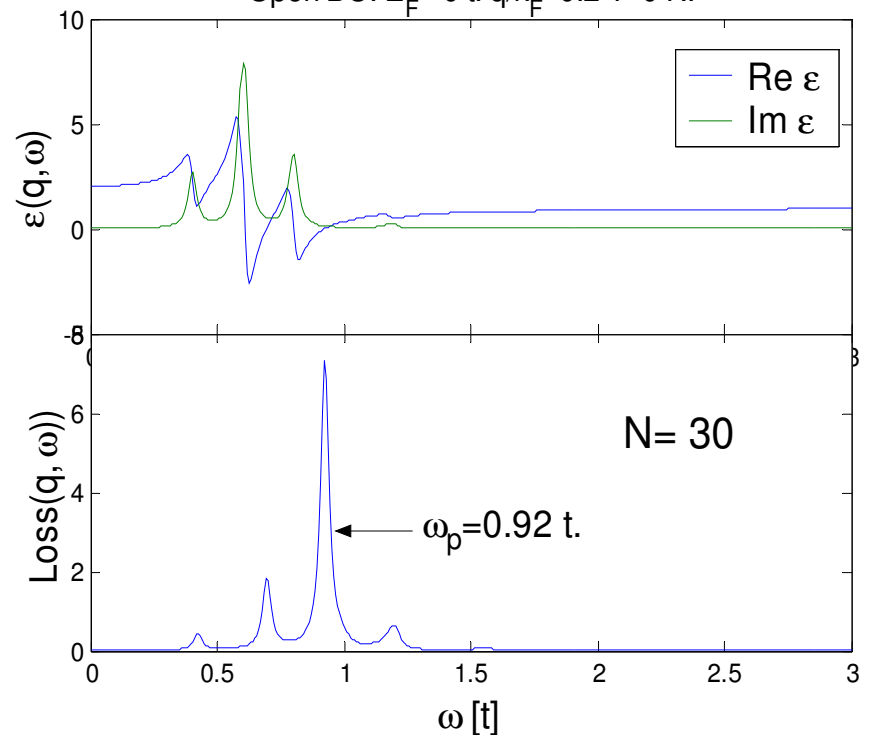
Plasmons

- Appear as peaks in the loss function. $Loss = \text{Im} \frac{-1}{\epsilon(\mathbf{q}, \omega)}$
- Occur when $\text{Re } \epsilon$ goes to zero and $\text{Im } \epsilon$ is small.

Dielectric and Loss Functions for a 1D Chain.
Open BC. $E_F = 0$ t. $q/k_F = 0.2$ T=0 K.

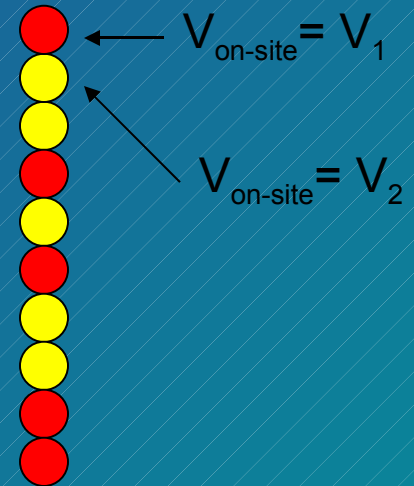


Dielectric and Loss Functions for a 1D Chain.
Open BC. $E_F = 0$ t. $q/k_F = 0.2$ T=0 K.



Optimal Design

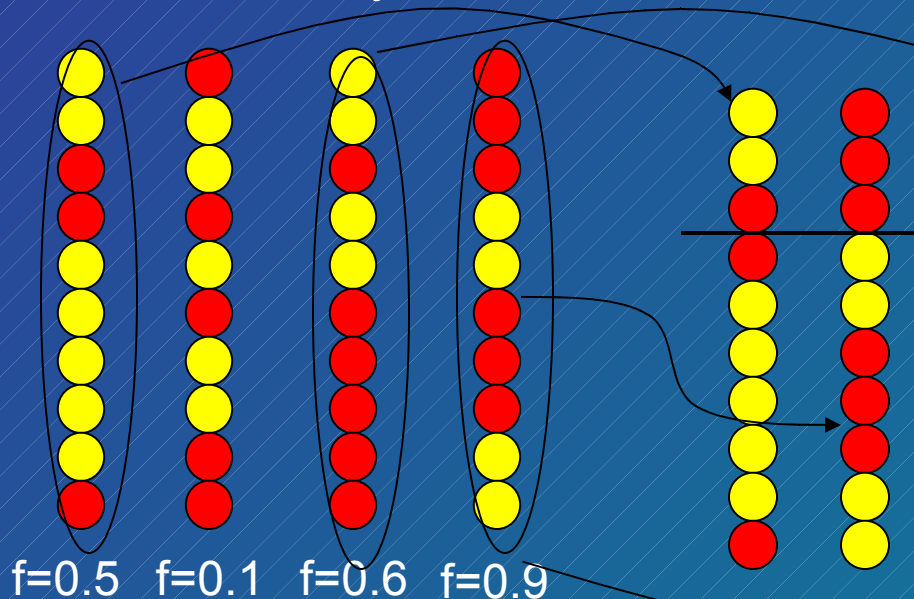
- Target:
 - Loss function with resonance peak at desired frequency
- System:
 - 1D Chain of two different species of atoms with different on-site-potentials
- Genetic Algorithm
 - Optimization algorithms based on natural selection
 - Advantages:
 - Easy to implement
 - Avoid getting trapped in local minima
 - Scalable



Genetic Algorithm Procedure

1. Initialization:

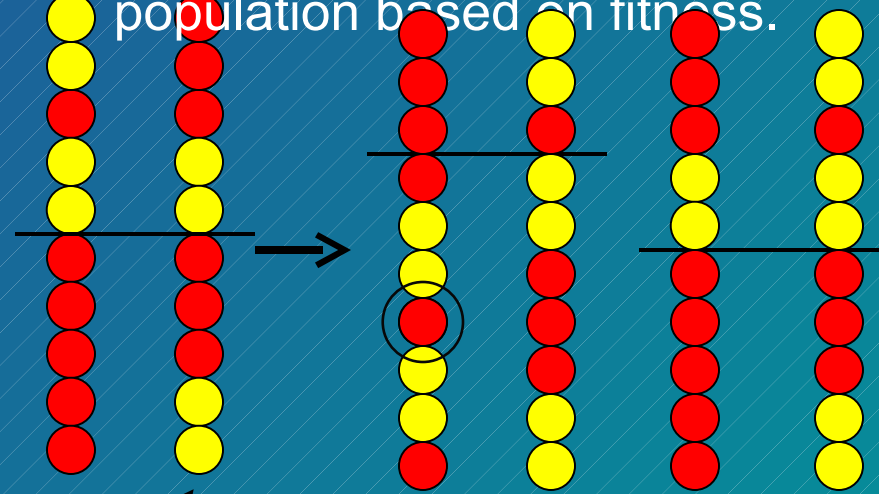
- Randomly create chains



1. Selection:

- Calculate fitness values, $f \in [0,1]$.

- Copy individuals from the population based on fitness.



1. Crossover:

- Cut two chains at random
- Swap the atoms between the two chains

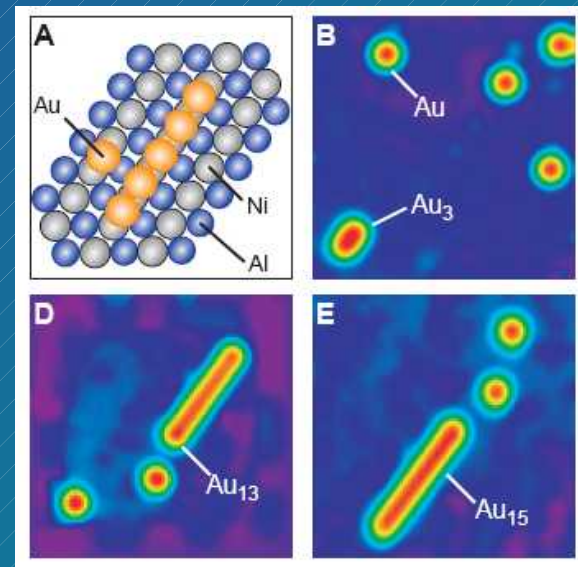
4. Mutation:

- Randomly switch a small number of individual atoms

5. Repeat

Experimental Realizations

- Metallic Atomic Chains
 - Nilius, *et al*, studied chains of 2-20 Au atoms on Ni/Al(110),
 - use a scanning tunneling microscope (STM) to manipulate individual atoms.¹
 - determined local electronic density of states from differential tunneling conductivity.
 - Similar studies on chains of Ag on Ni/Al(110)² and Cu on Cu(111)³
- Quasi-1D systems
 - Dielectric layers (GaAs, $\text{Al}_x\text{Ga}_{1-x}\text{As}$)



(A) Structure model of a Au_5 chain on NiAl(110).

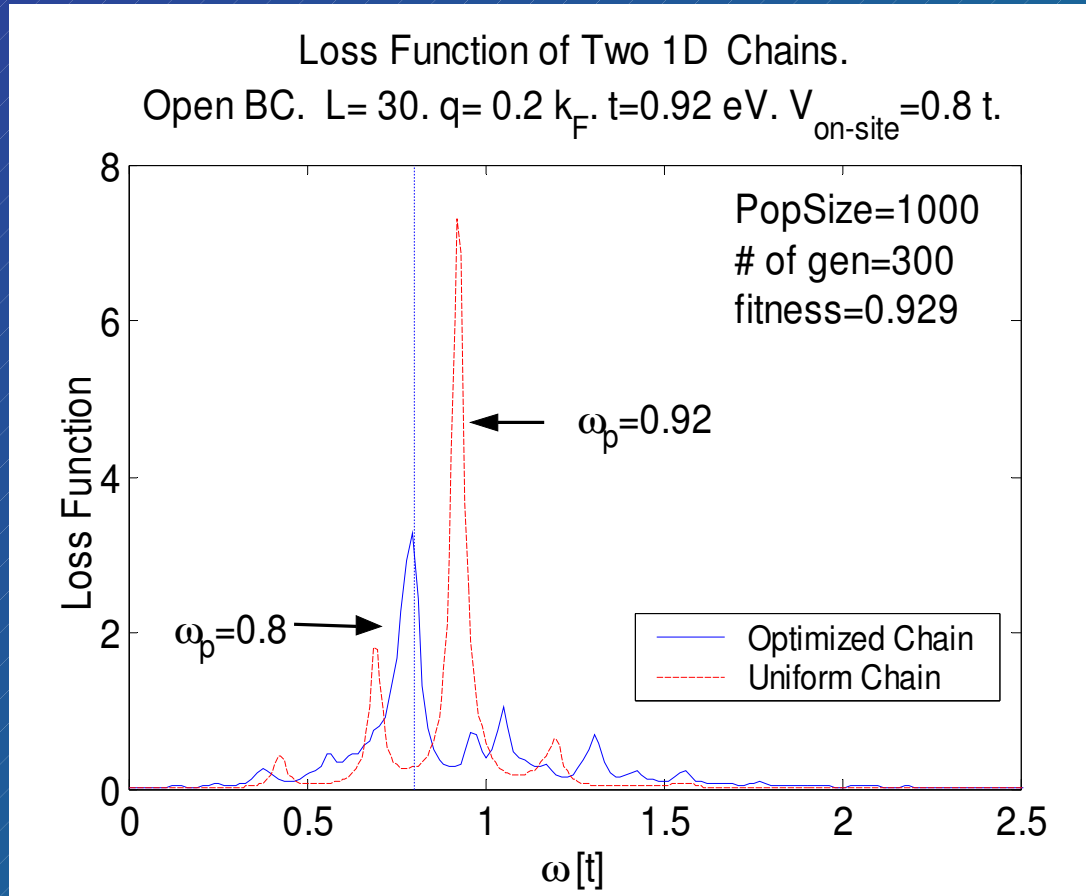
(B, D, E) STM images of Au chains. (image sizes 95 \AA by 95 \AA , $V_{\text{sample}} = 2.1 \text{ V}$, $I = 1 \text{ nA}$).¹

¹Nilius, *et al.* Science **297** 1853 (2002)

²Nazin, *et al.*, Phys. Rev. Lett. **90** 216110 (2003)

³Fölsch *et al.*, Phys. Rev. Lett. **92** 056803 (2004)

Loss Function of Optimized Chain, $\omega_p = 0.8 t$



Target:

$$\omega_p = 0.8 t \pm 0.3$$

- $V_{\text{on-site}} = 0 t$
- $V_{\text{on-site}} = 0.8 t$

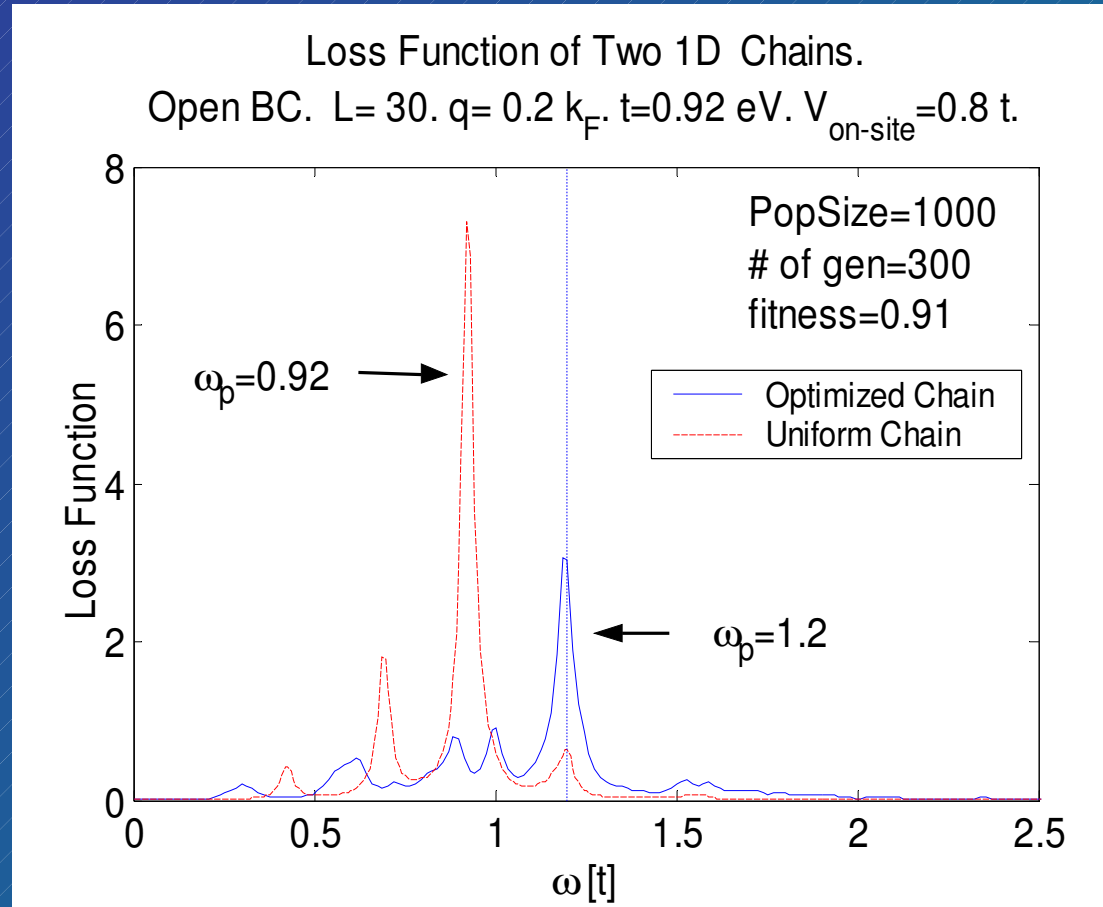


Optimized Chain



Uniform Chain

Loss Function of Optimized Chain, $\omega_p = 1.2 t$



Target:

$$\omega_p = 1.2 t \pm 0.3$$

- $V_{\text{on-site}} = 0 t$
- $V_{\text{on-site}} = 0.8 t$



Optimized Chain



Uniform Chain

Conclusions

- Summary
 - Developed a model to calculate plasmon modes of 1D systems.
 - Found chain sequences that match target plasmon resonances.
- Future applications in device design.
- Further Investigation:
 - Consider effects of substrate.
 - Consider chain with variable spacing between consecutive lattice sites.
 - Further develop physical model.

1D Tight-Binding Model

- Model 1D Chain with tight-binding Hamiltonian:

$$H = - \sum_{\langle i,j \rangle} t_{i,j} \left(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i \right) + \sum_i \mu_i n_i$$

- where:
 - $\langle i,j \rangle$ indicate a sum over nearest neighbors only
 - c_i^\dagger , c_j = creation, annihilation operators
 - $t_{i,j}$ = hopping integral between sites i,j
 - μ_i = on-site potential